Derivation of the Gross-Pitaevskii Equation
for Rotating Bose Gases

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Abstract

We prove that the Gross-Pitaevskii equation correctly describes the ground state energy and corresponding one-particle density matrix of rotating, dilute, trapped Bose gases with repulsive two-body interactions. We also show that there is 100% Bose-Einstein condensation. While a proof that the GP equation correctly describes non-rotating or slowly rotating gases was known for some time, the rapidly rotating case was unclear because the Bose (i.e., symmetric) ground state is *not* the lowest eigenstate of the Hamiltonian in this case. We have been able to overcome this difficulty with the aid of coherent states. Our proof also conceptually simplifies the previous proof for the slowly rotating case. In the case of axially symmetric traps, our results show that the appearance of quantized vortices causes spontaneous symmetry breaking in the ground state.

Dedicated to Jakob Yngvason on the occasion of his 60th birthday

1 Introduction

In this paper we show that a dilute, rotating Bose gas is correctly described by the Gross-Pitaevskii (GP) equation. We also show that there is 100% Bose-Einstein condensation (BEC) into a solution of the GP equation in a suitable limit. These conclusions were heretofore unproved, and it might not be an exaggeration to say that they were even conjectural, primarily because of the unusual situation (proved in [23]) that the absolute ground state of

the Schrödinger Hamiltonian is *not the bosonic ground state* in the rapidly rotating case, as it is in the case when there is little or no rotation. In other words, the vortices seen in rotating gases are not properties of the absolute ground state but are, instead, true manifestations of the bosonic symmetry requirement.

If the GP equation correctly describes the physics of a rotating gas (as we show here), then it also shows the superfluidity of such a gas, as will be discussed below. In the case of a cylindrically symmetric trap potential, the rotational symmetry is broken when more than one vortex is present; the GP equation must describe this broken rotational symmetry and, therefore, it must have multiple minimum energy solutions in this case.

The key mathematical tool employed here is coherent states. Our work is based on the results of [18] and the observation there that one can make a *c*-number substitution for many boson modes (not just one, as in Bogoliubov's method) without significant error provided the number of such modes is of lower order than N, the number of particles.

As in our previous work [15, 12, 17, 23, 14] on dilute, trapped Bose gases we start with the Hamiltonian for N bosons

$$H_N = \sum_{i=1}^{N} H_0^{(i)} + \sum_{1 \leq i < j \leq N} v_N (x_i - x_j), \tag{1}$$

where H_0 is the one-body part of the Hamiltonian and v_N is the two-body repulsive interaction. These terms and the GP limit are described as follows.

1. The GP limit: We want to fix the external trapping potential but let N tend to infinity. To retain the notion of a dilute gas in this situation we let the interparticle potential depend on N in such a way that a_N, the two-body scattering length of v_N, is related to N by the condition that

$$Na_N = a \qquad \text{is fixed.} \tag{2}$$

In this limit the three components of the energy (kinetic, trapping potential and interaction potential) scale in the same way and are all of the same order of magnitude. We call this the *GP limit*. It is this limit that will lead to the GP equation (6).

2. The two-body potential: We choose a radial two-body potential $w(x)$ such that $w(x) \geq 0$ (this is an important restriction for our methods) and such that $w(x) = 0$ for $|x| > R_0$ (this finite range condition is a technical restriction for simplicity and can be relaxed if need be). We note that integrability of $w(x)$ is not assumed here, $w(x)$ is even allowed to have a hard core. The scattering length of w is a (i.e., the solution to $[-\frac{1}{2}\Delta + w(x)]f(x) = 0$ with $f(\infty) = 1$ satisfies $f = 1 - a/|x|$ for $|x| > R_0$). The actual two-body potential in (1), given by

$$v_N(x) = N^2 w(Nx), \tag{3}$$

has scattering length $a_N = a/N$.

3. The one-body Hamiltonian: We work, as usual, in the rotating coordinate system, in which case the kinetic energy has to be supplemented by a term $-\Omega \cdot (p \wedge x) = p \cdot (\Omega \wedge x)$, where Ω is the angular velocity vector, and $p = -i\hbar\nabla$. It is convenient to add and subtract

a term $\frac{m}{2}(\Omega \wedge x)^2$ and thereby write

$$H_0 = \frac{1}{2m}(p + A(x))^2 + V(x) \tag{4}$$

with $A(x) = m\Omega \wedge x$. Then V is the trapping potential (which might or might not have some geometric symmetry) *minus* $\frac{m}{2}(\Omega \wedge x)^2$. It is well known that we must have $V(x) \to \infty$ as $|x| \to \infty$, for otherwise the system will fly apart. We can also assume that $V \geq 0$ without loss of generality. Actually, for technical reasons we require just a little more, namely $V(x) \geq C_1 \ln(|x|) - C_2$ for some positive constants C_1 and C_2. (This condition can probably be relaxed a bit. What we actually need is that $\text{Tr}\, e^{\alpha(\Delta - V(x))}$ and $\text{Tr}\, |A(x)|^s e^{\alpha(\Delta - V(x))}$ are finite for α large enough, for some $s > 2$. We will show in the appendix that this is fulfilled under the stated assumption on V.)

We note that in the rotating coordinate system, the velocity at x is not p/m but rather $v = i\hbar^{-1}[H_0, x] = p/m + \Omega \wedge x$. The angular velocity around the Ω axis is $\Omega \cdot (v \wedge x)|x^\perp|^{-2}|\Omega|^{-1}$, where $|x^\perp|$ is the distance to the Ω axis. In a cylindrically symmetric state ψ we have $\Omega \cdot (p \wedge x)\, \psi = 0$ and, therefore, the angular velocity is Ω, not zero. In the *fixed* frame the angular velocity is $\Omega - \Omega = 0$. In other words, the system in such a state is not rotating. As long as Ω is small enough, the GP ground state is cylindrically symmetric and hence there is no rotation; this is a manifestation of superfluidity. In order to have rotation at least one vortex must form. This is a typical property of superfluids.

Henceforth, we use units in which $\hbar = 2m = 1$. We also note that the modification of the kinetic energy in (4) is mathematically just like that caused by a uniform magnetic field with vector potential A (and $e/c = 1$). There is nothing special about $A(x) = m\Omega \wedge x$ as far as the mathematics is concerned, so one could have an arbitrary A without disturbing our analysis, provided it did not grow too fast at infinity. One could think, for example, of applying a magnetic field to the system, but then our particles would have to be charged and the attendant Coulomb interaction would nullify the treatment of the system as a dilute gas with short range interaction. On the other hand, we could allow our particles to have a magnetic moment ("bosons with spin") and our analysis would easily extend to this case. The ground state energy depends in a non-trivial way on the total spin when there is rotation [22], even in the absence of a magnetic field. This is due to the symmetry requirement of the wave function, whereby the symmetry of the spin part determines the spatial symmetry (see, e.g., [6]). We will not pursue this topic further in this paper.

Our analysis is carried out here for three-dimensional gas particles, but the same ideas apply to a two-dimensional gas. There will be changes, of course, because the notion of scattering length is different in 2D and because the energy per particle of a homogeneous gas of low density ϱ is not $4\pi\varrho a_s$ as in 3D but rather $4\pi\varrho/|\log \varrho a_s^2|$. (Here, a_s is the unscaled scattering length of the interaction potential, which is held fixed in the thermodynamic limit for the homogeneous gas.) Thus, the GP equation will be a little different, but the conclusion will be the same: The only effect of rotation is to replace p^2 by $|p + A|^2$ in the GP equation derived in [16]. In order to keep this paper manageable we do not discuss the 2D case, but the interested reader can easily combine the results in [16], [23] and the present paper.

The Hamiltonian H_N acts on $L^2(\mathbb{R}^{3N})$ but we are interested in its restriction to the *bosonic* subspace of $L^2(\mathbb{R}^{3N})$, namely to permutation symmetric functions. We denote the ground state energy of H_N in the bosonic sector by $E_0(N)$, and we keep in mind that this might be larger than the absolute ground state energy of H_N when no permutation symmetry is imposed.

We turn now to the GP equation, which originates from the GP energy functional for a complex-valued function ϕ of one variable $x \in \mathbb{R}^3$. For $a \geq 0$, the GP energy functional is given by

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \langle\phi|H_0|\phi\rangle + 4\pi a \int_{\mathbb{R}^3} |\phi(x)|^4 dx \ . \tag{5}$$

It can easily be shown [15] that $\mathcal{E}^{\mathrm{GP}}[\phi]$ has a minimum over all ϕ with $\|\phi\|_2 = 1$ and this minimum energy is denoted by $E^{\mathrm{GP}}(a)$. (We use the standard notation $\|\phi\|_p = \left[\int |\phi(x)|^p \, dx\right]^{1/p}$.) There might be several minimizers (and there surely will be when the trap has axial symmetry and a is large [22, 23]) but each minimizing ϕ will satisfy the GP equation

$$(-i\nabla + A(x))^2\phi(x) + V(x)\phi(x) + 8\pi a|\phi(x)|^2\phi(x) = \mu\phi(x)\,, \tag{6}$$

where μ is the chemical potential (i.e., the energy per particle to add a small number of particles). Note that $\mu = E^{\mathrm{GP}}(a) + 4\pi a \int |\phi(x)|^4 dx > E^{\mathrm{GP}}(a)$ because of the quartic non-linearity.

Our main theorem concerning the bosonic ground state energy of (1) is the following.

Theorem 1. *With a denoting the scattering length of w, we have*

$$\lim_{N\to\infty} \frac{E_0(N)}{N} = E^{\mathrm{GP}}(a)\,. \tag{7}$$

In [23] it was shown that

$$\limsup_{N\to\infty} \frac{E_0(N)}{N} \leq E^{\mathrm{GP}}(a)\,, \tag{8}$$

and, therefore, it remains only to prove a lower bound to $\liminf_{N\to\infty} E_0(N)/N$ of the right form, which we do here.

The GP energy minimizer(s) ϕ also tells us something about the density (diagonal and off-diagonal) and about Bose-Einstein condensation in the ground state of H_N, or any *approximate ground state*. We call a *sequence* of bosonic N-particle density matrices γ_N an approximate ground state if $\lim_{N\to\infty} N^{-1}\mathrm{Tr}\, H_N\gamma_N = E^{\mathrm{GP}}(a)$. The reduced one-particle density matrix of γ_N will be denoted by $\gamma_N^{(1)}$.

We would like to suppose that, as $N \to \infty$, $\gamma_N^{(1)}$ converges to some γ and that $\gamma = |\phi\rangle\langle\phi|$, where ϕ is a solution to the GP equation. This would be 100% Bose-Einstein condensation into the GP state and was proved to occur in the non-rotating case [12]. The difficulty in the rotating case is that the solution to the GP equation might not be unique (as it is in the non-rotating case), in which case the limit γ need not be a pure state. We would expect, however, that γ is always a convex combination of pure GP states, i.e., $\gamma = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$,

where ϕ_i is a solution to the GP equation and $\sum_i \lambda_i = 1$. (This, of course, is not the same as the much weaker and less interesting statement that γ is a convex combination of terms of the form $|\psi\rangle\langle\psi|$, in which ψ is a linear combination of GP solutions instead of being equal to just one GP solution.) Unfortunately, as in the case of a cylindrically symmetric trap, the set of GP states might not be countable, and so the summation $\sum_i$ must be replaced by some kind of integral. This accounts for the rather abstract Theorem 2 below. In any event, this theorem tells us that there is always 100% condensation, even if the system has a wide choice of states into which to condense.

Note that $\gamma_N^{(1)}$ is a positive trace class operator on the one-particle space $L^2(\mathbb{R}^3)$, and we choose the normalization $\mathrm{Tr}\,\gamma_N^{(1)} = 1$ for convenience. (The conventional normalization is $\mathrm{Tr}\,\gamma_N^{(1)} = N$.) By the Banach-Alaoglu Theorem, any sequence $\gamma_N^{(1)}$ will have a subsequence that converges to some γ in the weak-* topology, i.e., $\lim_{N\to\infty} \mathrm{Tr}\, A\gamma_N^{(1)} = \mathrm{Tr}\, A\gamma$ for all compact operators A. This convergence will even hold in the norm topology, i.e., $\lim_{N\to\infty} \mathrm{Tr}\,|\gamma_N^{(1)} - \gamma| = 0$ by compactness. More precisely, since the $\gamma_N^{(1)}$ are the one-particle density matrices of approximate ground states, we have (using the positivity of the interaction potential in H_N) $\mathrm{Tr}\, H_0\gamma_N^{(1)} \leq$ const. independently of N. Hence also $\sqrt{H_0}\gamma_N^{(1)}\sqrt{H_0} \rightharpoonup \sqrt{H_0}\gamma\sqrt{H_0}$ in weak-* sense, i.e., $\mathrm{Tr}\, A\sqrt{H_0}\gamma_N^{(1)}\sqrt{H_0} \to \mathrm{Tr}\, A\sqrt{H_0}\gamma\sqrt{H_0}$ for all compact A. Since H_0^{-1} is a compact operator, this implies that $\mathrm{Tr}\,\gamma_N^{(1)} \to \mathrm{Tr}\,\gamma$ as $N \to \infty$ (simply use $A = H_0^{-1}$ above). For positive operators, weak-* convergence plus convergence of the trace implies norm-convergence [27, 25].

We denote by Γ the set of all $\gamma's$ that are limit points of one-particle density matrices of approximate minimizers. That is,

$$\Gamma = \left\{ \gamma \,:\, \text{there is a sequence } \gamma_N,\ \lim_{N\to\infty} \frac{1}{N}\mathrm{Tr}\, H_N\gamma_N = E^{\mathrm{GP}}(a),\ \lim_{N\to\infty} \gamma_N^{(1)} = \gamma \right\}. \quad (9)$$

As remarked above, the convergence $\gamma_N^{(1)} \to \gamma$ can either mean weak-* convergence or norm convergence. Note that, in particular, norm convergence implies that $\mathrm{Tr}\,\gamma = 1$ for all $\gamma \in \Gamma$.

Theorem 2. *The set Γ of one-particle density matrices of approximate ground states, as defined in (9), has the following properties.*

  (i) Γ is a compact and convex subset of the set of all trace class operators.

  (ii) Let $\Gamma_{\mathrm{ext}} \subset \Gamma$ denote the set of extreme points in Γ. (An element $\gamma \in \Gamma$ is <u>extreme</u> if γ cannot be written as $\gamma = a\gamma_1 + (1-a)\gamma_2$ with $\gamma_{1,2} \in \Gamma$, $\gamma_1 \neq \gamma_2$, and $0 < a < 1$.) We have $\Gamma_{\mathrm{ext}} = \{|\phi\rangle\langle\phi| \,:\, \mathcal{E}^{\mathrm{GP}}[\phi] = E^{\mathrm{GP}}(a)\}$, i.e., the extreme points in Γ are given by the rank-one projections onto GP minimizers.

  (iii) For each $\gamma \in \Gamma$, there is a positive (regular Borel) measure $d\mu_\gamma$, supported in Γ_{ext}, with $\int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi) = 1$, such that

$$\gamma = \int_{\Gamma_{\mathrm{ext}}} d\mu_\gamma(\phi)\, |\phi\rangle\langle\phi|, \quad (10)$$

where the integral is understood in the weak sense. That is, every $\gamma \in \Gamma$ is a convex combination of rank-one projections onto GP minimizers.

A consequence of the Krein–Milman Theorem [4, vol. 2, Thm. 25.12] is that given any $\gamma \in \Gamma$ and given any $\varepsilon > 0$ there are finitely many GP minimizers ϕ_i and positive coefficients λ_i (with $\sum_i \lambda_i = 1$) such that

$$\gamma = \sum_i \lambda_i \, |\phi_i\rangle\langle\phi_i| + \Delta_\varepsilon \tag{11}$$

with $\mathrm{Tr}\, |\Delta_\varepsilon| < \varepsilon$. That is, every element of Γ can be approximated by a *finite* convex combination of GP minimizers. We also note that part (iii) of Theorem 2 follows from part (ii) using Choquet's Theorem [4, vol. 2, Thm. 27.6]. We shall, however, prove part (iii) (and Eq. (11)) directly in Section 3 (see Step 4).

Eq. (10) reflects the *spontaneous symmetry breaking* that occurs in the system under consideration. Consider the case of an external potential $V(x)$ which is axially symmetric, with symmetry axis given by the angular velocity vector Ω. In general, the non-uniqueness of the GP minimizer stems from the appearance of *quantized vortices*, which break the axial symmetry, and hence lead to a whole continuum of GP minimizers [22, 23, 2, 3, 8, 7, 1]. Uniqueness of the GP minimizer can be restored by perturbing the one-particle Hamiltonian H_0 in such a way as to break the symmetry and to favor one of the minimizers, e.g., by introducing a slightly asymmetric trap potential $V(x)$. This then leads to *complete BEC*, as can be seen from our Theorem 2, which does not assume any particular symmetry of $V(x)$. Note that in the case of a unique GP minimizer, Theorem 2 implies that the reduced one-particle density matrix of *any* approximate ground state converges to the projection onto this unique GP minimizer, since Γ_{ext} (and hence Γ) consists of only one element in this case.

The situation of a dilute rotating Bose gas described in this section contrasts with the situation of the *absolute* ground state of H_N, i.e., the lowest eigenvalue and corresponding state without imposing symmetry restrictions on the wavefunctions. In [23] it was shown that Eq. (7) does *not* hold, in general, for the absolute ground state energy. The energy per particle in this case is given by minimizing a functional similar to (5), but which now depends on one-particle density matrices rather than on wave functions $\phi(x)$. In [22, 23] it was shown that the corresponding energy is *strictly lower* than $E^{\mathrm{GP}}(a)$ for a large enough (and $\Omega \neq 0$). The density matrix functional has a *unique* minimizer for any value of Ω and a, and in general this minimizer will not be rank one. An analogue of Theorem 2 also holds for the absolute ground state. As shown in [23], Γ consists of only one element in this case, namely the unique minimizer of the density matrix functional just mentioned. This implies, in particular, that there is no spontaneous symmetry breaking in the absolute ground state. We refer the reader to [23] for more details.

In the remainder of this paper, we present the proof of Theorems 1 and 2.

2 Proof of Theorem 1

STEP 1. Reduction of the Number of Particles to Ensure a Bounded Energy per Particle.

One of the problems we shall face in our analysis is to control three-body collisions, i.e., to show that the ground state wave function is suitably small when three particles are close together. We have found a way to do this (see Step 4) with the help of a bound on the change in energy when three particles are added to the system. It is not evident that this bound is always satisfied (although it must be satisfied on average since the total energy is bounded by N) and the discussion in this subsection shows how to circumvent this annoyance. If another way could be found to control the three-body amplitude or to control the incremental energy then the analysis in this section would not be needed.

Let us consider the Hamiltonian (1) for $M \leq N$ particles (but still with interaction potential v_N depending on N):

$$H_{M,N} = \sum_{i=1}^{M} H_0^{(i)} + \sum_{1 \leq i < j \leq M} v_N (x_i - x_j) \,. \tag{12}$$

This operator acts naturally on all of $L^2(\mathbb{R}^{3M})$. We denote the ground state energy in the *bosonic* sector by $E_0(M, N)$. Our goal is a good lower bound on $E_0(N, N)$.

Let $\widetilde{M} = \widetilde{M}(N)$ be the largest integer $\leq N$ satisfying two conditions: a.) $N - \widetilde{M}$ is divisible by 3 and b.) $E_0(\widetilde{M}, N) - E_0(\widetilde{M} - 3, N) \leq 6 E^{\mathrm{GP}}(a)$. Then $E(\widetilde{M} + 3, N) - E(\widetilde{M}, N) > 6 E^{\mathrm{GP}}(a)$, $E(\widetilde{M} + 6, N) - E(\widetilde{M} + 3, N) > 6 E^{\mathrm{GP}}(a)$, etc., whence

$$E_0(N, N) \geq E_0(\widetilde{M}, N) + 2(N - \widetilde{M}) E^{\mathrm{GP}}(a) \,. \tag{13}$$

We will prove the following in the remainder of this section.

Proposition 1. *Fix $Z > 0$, and let M_j and N_j be two sequences of integers, with $M_j \leq N_j$, $\lim_{j \to \infty} M_j = \infty$ and $\lim_{j \to \infty} N_j = \infty$, such that $E_0(M_j, N_j) - E_0(M_j - 3, N_j) \leq 3Z$ for all j and $\lim_{j \to \infty} M_j / N_j = \lambda$ for some $0 \leq \lambda \leq 1$. Then*

$$\liminf_{j \to \infty} \frac{1}{N_j} E_0(M_j, N_j) \geq \lambda E^{\mathrm{GP}}(\lambda a) \,. \tag{14}$$

Note that (14) does not depend on Z.

It is now useful to note that the energy $E^{\mathrm{GP}}(a)$ is concave in a (as an infimum over affine functions) and thus satisfies

$$E^{\mathrm{GP}}(\lambda a) \geq (1 - \lambda) E^{\mathrm{GP}}(0) + \lambda E^{\mathrm{GP}}(a) \geq \lambda E^{\mathrm{GP}}(a) \,. \tag{15}$$

The last inequality in (15) follows from $E^{\mathrm{GP}}(0) > 0$.

The sequence $\widetilde{M}(N)$ defined above will have a subsequence such that $\widetilde{M}(N_j)/N_j \to \lambda$ as $j \to \infty$ for some $0 \leq \lambda \leq 1$. If we combine (13)–(15) with $Z = 2 E^{\mathrm{GP}}(a)$ we find for this sequence that

$$\lim_{j \to \infty} E_0(N_j, N_j)/N_j \geq \lambda^2 E^{\mathrm{GP}}(a) + 2(1 - \lambda) E^{\mathrm{GP}}(a) = [1 + (1 - \lambda)^2] E^{\mathrm{GP}}(a) \geq E^{\mathrm{GP}}(a) \,, \tag{16}$$

which proves (7) for this sequence N_j. (Here and in the following, we denote $\liminf$ by $\underline{\lim}$ for short.) Together with the upper bound (8) we also conclude from (16) that $\lambda = 1$. That is, for $Z \geq 2E^{\mathrm{GP}}(a)$ the sequence $\widetilde{M}(N)/N$ has only 1 as a limit point, and hence (16) holds for the full sequence $N = 1, 2, 3 \ldots$.

Our goal in the rest of this section is to prove Proposition 1, which then proves (7), as just explained.

STEP 2. The Generalized Dyson Lemma.

To get a lower bound on $E_0(M, N)$, we start by deriving a lower bound on the Hamiltonian $H_{M,N}$, using Corollary 1 in [13]. This corollary, which is a generalization of Lemma 1 in [19] which, in turn, stems from Lemma 1 in Dyson's paper [5], asserts the following. (Note that the range of the potential v_N is R_0/N, and its scattering length is a/N. We use the "hat" $\widehat{}$ to denote Fourier transform.)

Lemma 1. *Let $R > R_0/N$. Let $\chi(p)$ be a radial function such that $0 \leq \chi(p) \leq 1$ and such that $h(x) \equiv \widehat{(1-\chi)}(x)$ is bounded and integrable (which implies that $\chi(p) \to 1$ as $|p| \to \infty$). Let*

$$f_R(x) = \sup_{|y| \leq R} |h(x - y) - h(x)|, \tag{17}$$

and

$$w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} f_R(y) \, dy. \tag{18}$$

Let $U_R(x)$ be any positive, radial function that vanishes outside the annulus $R_0/N \leq |x| \leq R$, with $\int_{\mathbb{R}^3} U_R(x) \, dx = 4\pi$. Let $\varepsilon > 0$. If $y_1, \ldots, y_n$ denote n fixed points in $\mathbb{R}^3$, with $|y_i - y_j| \geq 2R$ for all $i \neq j$, then we have the operator inequality on $L^2(\mathbb{R}^3)$

$$-\nabla\chi(p)^2\nabla + \tfrac{1}{2}\sum_{i=1}^{n} v_N(x - y_i) \geq \sum_{i=1}^{n}\left((1-\varepsilon)\frac{a}{N}U_R(x - y_i) - \frac{a}{N\varepsilon}w_R(x - y_i)\right). \tag{19}$$

The sums in (19) are multiplication operators, i.e., they are just functions of x. The operator $-\nabla\chi(p)^2\nabla$ is just the positive multiplication by $p^2\chi(p)^2$ in Fourier space. The original Lemma 1 in [19] has $\chi(p) \equiv 1$ and $h = w_R = f = \varepsilon = 0$.

Clarification: What Lemma 1 really says is that we can replace the unpleasant interaction potential v_N (which possibly contains an infinite hard core) by a small, smooth, but longer ranged potential whose main part, U_R, is positive. There are two prices that have to be paid for this luxury. One is to forego a piece of the positive kinetic energy, $-\nabla\chi(p)^2\nabla$. The second is that the potential is really only a 'nearest neighbor' potential. That is to say, the particle at x is allowed to interact with only one other particle at a time. This is seen from the requirement that the interaction U_R has range R, but the other particles must be separated by a distance $2R$. In order to utilize the coherent state inequalities later on in Step 3 we have to extend our U_R to an ordinary two-body potential, i.e., we have to be able to drop the $2R$ separation requirement. To do so will require an estimation of the amplitude (in the exact, original ground state wave function) of finding three or more particles within

a distance $2R$ of each other. Clearly, this amplitude is small, but we find that we have to resort to path integrals (or, more precisely, the Trotter product formula) to estimate it. This will be done in Step 4 below.

As an immediate corollary of Lemma 1 we can omit the condition $|y_i - y_j| \geq 2R$ and replace (19) by

$$
- \nabla \chi(p)^2 \nabla + \tfrac{1}{2} \sum_{i=1}^{n} v_N (x - y_i)
$$
$$
\geq \sum_{i=1}^{n} \left[(1 - \varepsilon) \frac{a}{N} U_R(x - y_i) - \frac{a}{N\varepsilon} w_R(x - y_i) \right] \prod_{k \neq i} \theta(|y_k - y_i| - 2R) \tag{20}
$$

for any set of points $y_j \in \mathbb{R}^3$. Here, θ denotes the Heaviside step function, given by $\theta(t) = 1$ if $t \geq 0$ and $\theta(t) = 0$ if $t < 0$. That is to say, if there are only $n' < n$ of the y_i that are a distance $\geq 2R$ from all the other y_k then we simply apply (19) to these n' coordinates. The right side of (20) does not contain the other values of i because the $\prod \theta$ factor vanishes for those. The left side does contain these unwanted y_i but, since v_N is non-negative, this does no harm to the inequality (20).

We apply (20) to each particle, considering the other $M-1$ particles as fixed, and obtain

$$
H_{M,N} \geq \sum_{i=1}^{M} \left(-\nabla_i \left(1 - \chi(p_i)^2 \right) \nabla_i + 2 p_i \cdot A(x_i) + A(x_i)^2 + V(x_i) \right)
$$
$$
+ \sum_{i=1}^{M} \sum_{j \neq i} \left[(1 - \varepsilon) a N^{-1} U_R(x_i - x_j) - a(N\varepsilon)^{-1} w_R(x_i - x_j) \right] \prod_{k \neq i, j} \theta(|x_k - x_j| - 2R). \tag{21}
$$

For the negative part of the interaction (containing w_R), we can simply use $\prod \theta \leq 1$ for a lower bound. For the positive part (containing U_R), we will use the fact that

$$
\prod_{k \neq i, j} \theta(|x_k - x_j| - 2R) \geq 1 - \sum_{k \neq i, j} \theta(2R - |x_k - x_j|), \tag{22}
$$

which follows from the simple inequality $\prod_j (1 - s_j) \geq 1 - \sum_j s_j$ when $0 \leq s_j \leq 1$ for all j.

We now use (21) and (22) in the following way. We begin by defining a new M-particle Hamiltonian, K, by

$$
K = \sum_{i=1}^{M} K_0^{(i)} + \sum_{1 \leq i < j \leq M} 2(1 - \varepsilon) \, a N^{-1} U_R(x_i - x_j), \tag{23}
$$

where K_0 is a one-body Hamiltonian to be described next. If K_0 were simply $(-i\nabla + A)^2 + V$ then (23) would be the conventional Hamiltonian with two-body interaction $2U_R$. (The factor 2 arises because each pair i, j appears twice in (21).)

Unfortunately, K_0 has to be a little more complicated because we used up part of the kinetic energy in replacing v_N by U_R via Lemma 1. Pick some $\eta > 0$, and let

$$
K_0 = -\nabla \left(1 - \chi(p)^2 \right) \nabla - 2\eta \Delta + 2 p \cdot A(x) + A(x)^2 + V(x) + \eta |x|^4 - \kappa(\eta). \tag{24}
$$

The constant $\kappa(\eta)$ is chosen so that $K_0 > 0$. It is a matter of convenience to include it in the definition of K_0. It is defined by

$$\kappa(\eta) = \inf \mathrm{spec} \left[-\eta\Delta + 2p \cdot A(x) + \eta|x|^4\right]. \tag{25}$$

The reason for adding the terms $-2\eta\Delta$ and $\eta|x|^4$ to K_0 is to ensure that K_0 is bounded from below and has compact resolvent, and so that $\kappa(\eta)$ is finite. (Note: the exponent 4 in $|x|^4$ could be replaced by any exponent > 2 for our purposes. This is due to the fact that we have a vector potential $A(x)$ in mind that is bounded by $(\mathrm{const.})|x|$, as in the case of pure rotation. If this is not so (because an external magnetic field has been added) some polynomial of higher order than $|x|^4$ could be needed, but our analysis would continue to go through.)

Since there is a $2\eta\Delta$ in (24) and not just $\eta\Delta$ we have that $K_0 \geq -\eta\Delta + V(x) \geq -\eta\Delta \geq 0$, since $V(x) \geq 0$ by assumption. This will be convenient later.

Let $\langle \cdot \rangle_\mathcal{B}$ denote the M-particle *bosonic* ground state expectation for the *original* Hamiltonian $H_{M,N}$. Actually, it is convenient to take the zero temperature limit of the Gibbs state, which means that in case of a ground state degeneracy of $H_{M,N}$, we would take $\langle \cdot \rangle_\mathcal{B}$ to be the uniform average over all ground states. Then $E_0(M, N) = \langle H_{M,N} \rangle_\mathcal{B}$ and we have, therefore, using (21)–(25),

$$E_0(M, N) \geq \inf \mathrm{spec} \, K + M\kappa(\eta) - \eta M \langle |x_1|^4 \rangle_\mathcal{B} - 2\eta M \langle -\Delta_1 \rangle_\mathcal{B}$$
$$- \frac{M^2 a}{N\varepsilon} \langle w_R(x_1 - x_2) \rangle_\mathcal{B} - \frac{aM^3}{N} \langle U_R(x_1 - x_2)\theta(2R - |x_2 - x_3|) \rangle_\mathcal{B}. \tag{26}$$

(Note: We made use of the bosonic symmetry to replace $\sum_i \Delta_i$ by $M\Delta_1$, for example.)

The term $\langle -\Delta_1 \rangle_\mathcal{B}$ can be bounded as follows. We have $p^2 \leq 2(p + A)^2 + 2A^2$, and hence, using positivity of the interaction potential v_N,

$$M \langle -\Delta_1 \rangle_\mathcal{B} \leq 2E_0(M, N) + \tfrac{1}{2}|\Omega|^2 M \langle |x_1|^2 \rangle_\mathcal{B}. \tag{27}$$

To prove Proposition 1 we have to bound the various terms in (26) and (27), and that is what we do in the following steps. The main term to bound is $\inf \mathrm{spec} \, K$, the ground state energy of the 'effective Hamiltonian' (23).

The momentum cutoff $\chi(p)$ in (24) will be chosen as follows. Let $\ell(p)$ be an infinitely differentiable, spherically symmetric function with $\ell(p) = 0$ for $|p| \leq 1$, $\ell(p) = 1$ for $|p| \geq 2$ and $0 \leq \ell(p) \leq 1$ in-between. Then, for some adjustable parameter s to be determined later, we choose

$$\chi(p) = \ell(sp). \tag{28}$$

The potential $w_R(x)$ defined in (18) is then a smooth and rapidly decreasing function that depends only on the ratio R/s. It is easy to see that

$$\int_{\mathbb{R}^3} w_R(x)dx \leq \mathrm{const.} \frac{R^2}{s^2} \tag{29}$$

as long as $R \leq \mathrm{const.} \, s$. We will, in fact, choose $R \ll s$.

Finally, we are still free to make a choice for the function $U_R(x)$ in Lemma 1. We choose it to be a 'hat' function:

$$U_R(x) = \begin{cases} 6R^{-3} & R \geq |x| \geq 2^{-1/3}R \\ 0 & \text{otherwise}, \end{cases} \tag{30}$$

assuming that $R \geq 2^{1/3}R_0/N$, a condition that will be amply satisfied by our choice $N^{-1/3} \gg R \gg N^{-2/3}$ later on. We remark that the exact form of $U_R(x)$ is unimportant in what is to come. We will need only the properties that $\int U_R(x)dx = 4\pi$ and that $\|U_R\|_\infty \leq \text{const.}\, R^{-3}$ for $R \gg R_0/N$.

STEP 3. Coherent State Method for the Ground State.

We begin our analysis of (26) by bounding the main term, $\inf \operatorname{spec} K$. This will be done with the aid of coherent states, exploiting ideas in [18], and is, perhaps, the most methodologically novel part of our work.

The one-body operator K_0 has purely discrete spectrum and can be written in terms of its eigenvalues e_j and orthonormal eigenfunctions $|\varphi_j\rangle$ as $K_0 = \sum_{j \geq 1} e_j |\varphi_j\rangle\langle\varphi_j|$. Recall that $K_0 \geq -\eta\Delta + V(x) \geq -\eta\Delta \geq 0$, so $e_j > 0$. We assume the sequence e_j to be ordered, i.e., $e_{j+1} \geq e_j$ for all j. For simplicity, we introduce the notation

$$W(x_1 - x_2) \equiv (1 - \varepsilon)aN^{-1}U_R(x_1 - x_2). \tag{31}$$

The well known second quantization formalism involves the operators $a_j^\dagger$ and a_j which are the creation and annihilation operators of a particle in the state $|\varphi_j\rangle$. They satisfy the usual canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$, etc. The second quantized version of (23) is

$$\widehat{\mathcal{K}} = \sum_{j \geq 1} e_j a_j^\dagger a_j + \sum_{ijkl} a_i^\dagger a_j^\dagger a_k a_l W_{ijkl}, \tag{32}$$

where $W_{ijkl} = \langle\varphi_i \otimes \varphi_j|W|\varphi_k \otimes \varphi_l\rangle$. The operator $\widehat{\mathcal{K}}$ acts on the bosonic Fock space, $\mathcal{F}$, consisting of a direct sum over all particle number sectors. We are interested in a lower bound to the ground state energy of $\widehat{\mathcal{K}}$ in the sector of particle number M. Hence we can add a term $(\sum_j a_j^\dagger a_j - M)^2$ to $\widehat{\mathcal{K}}$ without changing this energy. We can then look for a lower bound *irrespective of particle number*. I.e., for any $C \geq 0$, we have that $\inf \operatorname{spec}\widehat{\mathcal{K}}$ for M particles is $\geq \inf \operatorname{spec}\mathcal{K}$ on the *full* Fock space, where

$$\mathcal{K} \equiv \sum_{j \geq 1} e_j a_j^\dagger a_j + \sum_{ijkl} a_i^\dagger a_j^\dagger a_k a_l W_{ijkl} + \frac{C}{M}\Big(\sum_{j \geq 1} a_j^\dagger a_j - M\Big)^2. \tag{33}$$

The choice of C will be made later.

The Fock space $\mathcal{F}$ can be thought of as the tensor product of the Fock spaces generated by each mode φ_j. We choose some integer $J \gg 1$ (to be determined later) and split the Fock space into two parts, namely $\mathcal{F} = \mathcal{F}^< \otimes \mathcal{F}^>$, where $\mathcal{F}^<$ is the tensor product of the Fock spaces generated by all the modes φ_j with $j \leq J$ and where $\mathcal{F}^>$ is that generated by all the other modes.

Next, we introduce coherent states [10] for all the modes $j \leq J$. (By coherent states we mean ordinary canonical Schrödinger, Bargmann, Glauber, coherent states.) The modes with $j > J$ will not be omitted, but they will be treated differently from the $j \leq J$ modes. Let $\mathbf{z} = (z_1, \ldots, z_J)$ denote a vector in $\mathbb{C}^J$. Let also $\Pi(\mathbf{z})$ denote the projection onto the coherent state $|z_1 \otimes \cdots \otimes z_J\rangle \in \mathcal{F}^<$. The symbol $|z_1 \otimes \cdots \otimes z_J\rangle$ is shorthand for $|z_1\rangle \otimes |z_2\rangle \otimes \cdots \otimes |z_J\rangle$, and $|z_j\rangle$ denotes the coherent state for the jth mode given by $|z_j\rangle = \exp[-|z_j|^2/2 + z_j a_j^\dagger]\,|\text{vacuum}\rangle$.

The Hamiltonian $\mathcal{K}$ in (33) can now be written as

$$\mathcal{K} = \int d\mathbf{z}\,\Pi(\mathbf{z}) \otimes U(\mathbf{z})\,, \tag{34}$$

where $U(\mathbf{z})$ is an operator acting on $\mathcal{F}^>$. The operator $U(\mathbf{z})$ depends on $\mathbf{z}$ since it is also an *upper symbol* for the modes $j \leq J$. The integration measure is $d\mathbf{z} = \pi^{-J} \prod_{j \leq J} dx_j dy_j$ with $z_j = x_j + iy_j$. This is discussed in [18, 10]. As an example, the upper symbol for $a_j^\dagger$ is $\bar{z}_j$ and for a_j it is z_j, but for $a_j^\dagger a_j$ it is $|z_j|^2 - 1$. Thus, to a term such as $a_i^\dagger a_j^\dagger a_k a_l$ with $i, j \leq J$ and $k, l > J$ would correspond the upper symbol operator $\bar{z}_i\,\bar{z}_j\,a_k a_l$.

It is easier to compute the *lower symbol* (which is denoted by $u(\mathbf{z})$) than the upper symbol $U(\mathbf{z})$. It is obtained simply by replacing $a_j^\dagger$ by $\bar{z}_j$ and a_j by z_j in all (normal-ordered) polynomials, even in higher polynomials such as $a_j^\dagger a_j$ or $a_j^\dagger a_j^\dagger a_j a_j$. An equivalent definition of the lower symbol of any polynomial $\mathcal{P}$ in the a_j's and $a_j^\dagger$'s (normal-ordered or not) is the expectation value $u(\mathbf{z}) = \langle z_1 \otimes \cdots \otimes z_J | \mathcal{P} | z_1 \otimes \cdots \otimes z_J \rangle$. In the case considered here, $u(\mathbf{z}) = \langle z_1 \otimes \cdots \otimes z_J | \mathcal{K} | z_1 \otimes \cdots \otimes z_J \rangle$.

The lower symbol is useful because the upper symbol can conveniently be obtained from it as [10]

$$U(\mathbf{z}) = e^{-\partial_\mathbf{z} \partial_{\bar{\mathbf{z}}}} u(\mathbf{z}) = u(\mathbf{z}) - \partial_\mathbf{z} \partial_{\bar{\mathbf{z}}} u(\mathbf{z}) + \tfrac{1}{2}\left(\partial_\mathbf{z} \partial_{\bar{\mathbf{z}}}\right)^2 u(\mathbf{z})\,, \tag{35}$$

where $\partial_\mathbf{z} \partial_{\bar{\mathbf{z}}} = \sum_{j \leq J} \partial_{z_j} \partial_{\bar{z}_j}$. (In the general case there would be higher order derivatives on the right side of (35), but not in our case since $u(\mathbf{z})$ is a polynomial of order four.) Note that (34) implies that

$$\inf \operatorname{spec} \mathcal{K} \geq \inf_{\mathbf{z}} \left(\inf \operatorname{spec} U(\mathbf{z})\right)\,, \tag{36}$$

since $\int d\mathbf{z}\,\Pi(\mathbf{z}) = \mathbb{I}_{\mathcal{F}^<}$ and $\Pi(\mathbf{z}) \otimes U(\mathbf{z}) \geq [\inf \operatorname{spec} U(\mathbf{z})]\,\Pi(\mathbf{z})$.

Our goal in the rest of this subsection is to derive a lower bound to $\inf \operatorname{spec} U(\mathbf{z})$ for a fixed $\mathbf{z}$. The reader might wonder why we use coherent states only for modes $j \leq J$ and not for all modes. The reason is that the upper symbol for the operator $e_j a_j^\dagger a_j$ is $e_j(|z_j|^2 - 1)$, and the -1 term is a term that we do not want when minimizing for a fixed $\mathbf{z}$. We make an error in the energy of the form $-\sum_{j \leq J} e_j$ and for this reason we cannot take $J = \infty$. But we can, and will let $J \to \infty$ as $N \to \infty$.

3a. Lower Bound on the Lower Symbol $u(\mathbf{z})$.

In order to derive a lower bound to $U(\mathbf{z})$ and the bottom of its spectrum, we start by deriving a lower bound to the lower symbol $u(\mathbf{z})$, which is the first term in (35). This symbol can be conveniently expressed in terms of the function $\Phi_\mathbf{z} \in L^2(\mathbb{R}^3)$, parametrized by $\mathbf{z} \in \mathbb{C}^J$,

given by

$$\Phi_{\mathbf{z}}(x) = \sum_{1 \leq j \leq J} z_j \varphi_j(x) \,. \tag{37}$$

Note that $\|\Phi_{\mathbf{z}}\|_2^2 = \sum_{j \leq J} |z_j|^2$.

Denoting $T \equiv \sum_{k > J} e_k a_k^\dagger a_k$, we have

$$\left\langle z_1 \otimes \cdots \otimes z_J \left| \sum_j e_j a_j^\dagger a_j \right| z_1 \otimes \cdots \otimes z_J \right\rangle = \sum_{j \leq J} e_j |z_j|^2 + T = \langle \Phi_{\mathbf{z}} | K_0 | \Phi_{\mathbf{z}} \rangle + T \,. \tag{38}$$

There is a mild abuse of notation here, which will continue for the rest of this paper, and which we hope will not cause any confusion. The operator $\sum_j e_j a_j^\dagger a_j$ acts on $\mathcal{F}$ while the vector $|z_1 \otimes \cdots \otimes z_J\rangle$ is in $\mathcal{F}^<$, so the left side of (38) defines an operator on $\mathcal{F}^>$ in an obvious way (actually, it defines a quadratic form). The right side must also be an operator on $\mathcal{F}^>$, and it is so if the number $\langle \Phi_{\mathbf{z}} | K_0 | \Phi_{\mathbf{z}} \rangle$ is regarded as a number times the identity on $\mathcal{F}^>$.

Similarly, with $N^> \equiv \sum_{j > J} a_j^\dagger a_j$ denoting the number of particles in the modes $> J$,

$$\left\langle z_1 \otimes \cdots \otimes z_J \left| \left(\sum_j a_j^\dagger a_j - M \right)^2 \right| z_1 \otimes \cdots \otimes z_J \right\rangle = \left(N^> + \|\Phi_{\mathbf{z}}\|_2^2 - M \right)^2 + \|\Phi_{\mathbf{z}}\|_2^2$$

$$\geq \left(\|\Phi_{\mathbf{z}}\|_2^2 - M \right)^2 - 2 e_J^{-1} M T \,. \tag{39}$$

Here, we used the normal ordering $[\sum_{j \leq J} a_j^\dagger a_j]^2 = \sum_{i \leq J} \sum_{j \leq J} a_i^\dagger a_j^\dagger a_i a_j + \sum_{j \leq J} a_j^\dagger a_j$, followed by the elementary bound $N^> \leq T/e_J$.

The interaction part of $u(\mathbf{z})$ is obtained by replacing a_j by z_j and $a_j^\dagger$ by $\bar{z}_j$ when $j \leq J$. We will now derive a lower bound on this term. It is convenient to introduce the notation

$$I(\Phi_{\mathbf{z}}) = \int dx dy \, |\Phi_{\mathbf{z}}(x)|^2 |\Phi_{\mathbf{z}}(y)|^2 W(x - y) \,. \tag{40}$$

Since $W \geq 0$, it is possible to neglect the interaction between modes $> J$ for a lower bound. More precisely, let $P = \sum_{1 \leq i \leq J} |\varphi_i\rangle\langle\varphi_i|$ and $Q = 1 - P$. The two-body operator $W(x - y)$ is then bounded from below by

$$\begin{aligned} W &= ((P + Q) \otimes (P + Q)) W ((P + Q) \otimes (P + Q)) \\ &\geq (P \otimes P) W (P \otimes P) + (P \otimes P) W (P \otimes Q + Q \otimes P + Q \otimes Q) \\ &\quad + (P \otimes Q + Q \otimes P + Q \otimes Q) W (P \otimes P) \,, \end{aligned} \tag{41}$$

since the missing term on the right side of (41) is $(Q \otimes Q + P \otimes Q + Q \otimes P) W (Q \otimes Q + P \otimes Q + Q \otimes P) \geq 0$. We thus have that

$$\left\langle z_1 \otimes \cdots \otimes z_J \left| \sum_{ijkl} a_i^\dagger a_j^\dagger a_k a_l W_{ijkl} \right| z_1 \otimes \cdots \otimes z_J \right\rangle$$

$$\geq I(\Phi_{\mathbf{z}}) + \sum_{kl > J} \langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} | W | \varphi_k \otimes \varphi_l \rangle a_k a_l + \sum_{kl > J} \langle \varphi_k \otimes \varphi_l | W | \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} \rangle a_k^\dagger a_l^\dagger$$

$$+ 2 \sum_{k > J} \langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} | W | \Phi_{\mathbf{z}} \otimes \varphi_k \rangle a_k + 2 \sum_{k > J} \langle \Phi_{\mathbf{z}} \otimes \varphi_k | W | \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} \rangle a_k^\dagger \,. \tag{42}$$

Here we used that W is symmetric, implying that in the last line we could replace $|\Phi_{\mathbf{z}} \otimes \varphi_k + \varphi_k \otimes \Phi_{\mathbf{z}}\rangle$ by $2|\Phi_{\mathbf{z}} \otimes \varphi_k\rangle$.

We seek a lower bound to the last two expressions in (42). Note that, for a general operator A, $|A + A^\dagger|^2 = A^2 + A^{\dagger 2} + AA^\dagger + A^\dagger A \le 2A^\dagger A + 2AA^\dagger$ by Schwarz's inequality, and so

$$(A + A^\dagger)^2 \le 4|A|^2 + 2[A, A^\dagger]. \tag{43}$$

We apply this to the second line in (42), with $A = \sum_{kl>J} c_{kl} a_k a_l$ and $c_{kl} = \langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}}|W|\varphi_k \otimes \varphi_l\rangle$. The commutator is

$$[A, A^\dagger] = 4 \sum_{klm>J} a_k^\dagger a_l \overline{c_{km}} c_{lm} + 2 \sum_{kl>J} |c_{kl}|^2. \tag{44}$$

The last term in (44) is bounded by

$$\sum_{kl>J} |c_{kl}|^2 \le \sum_{kl\ge1} |c_{kl}|^2 = \langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}}|W^2|\Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}}\rangle \le \|W\|_\infty I(\Phi_{\mathbf{z}}). \tag{45}$$

The first term on the right side of (44) can be bounded as

$$\sum_{klm>J} a_k^\dagger a_l \overline{c_{km}} c_{lm} \le \sum_{m\ge1} \sum_{kl>J} a_k^\dagger a_l \overline{c_{km}} c_{lm} \le \frac{4}{27\pi^4} \eta^{-1} \|W\|_1^2 \|\nabla\Phi_{\mathbf{z}}\|_2^4 T. \tag{46}$$

This can be seen as follows. The integral kernel σ of the one-particle operator defined by the matrix $\sum_{m\ge1} \overline{c_{km}} c_{lm}$ is given by

$$\sigma(x, x') = \int dy |\Phi_{\mathbf{z}}(y)|^2 W(x-y) W(x'-y) \overline{\Phi_{\mathbf{z}}(x)} \Phi_{\mathbf{z}}(x'). \tag{47}$$

Using Young's and Schwarz's inequalities, we have, for any function f on $\mathbb{R}^3$,

$$\int dx\, dx' \overline{f(x)} f(x') \sigma(x, x') \le \int dx\, dx'\, dy |\Phi_{\mathbf{z}}(y)|^2 W(x-y) W(x'-y) |\Phi_{\mathbf{z}}(x) f(x)|^2$$
$$\le \|W\|_1^2 \|\Phi_{\mathbf{z}}\|_6^2 \|\Phi_{\mathbf{z}} f\|_3^2 \le \|W\|_1^2 \|\Phi_{\mathbf{z}}\|_6^4 \|f\|_6^2. \tag{48}$$

Hence (46) follows by applying the Sobolev inequality $\|f\|_6^2 \le (4/3)(2\pi^2)^{-2/3} \|\nabla f\|_2^2$ both to f and to $\Phi_{\mathbf{z}}$, and using the fact that $-\Delta \le \eta^{-1} K_0$.

To get an upper bound on $|A|^2$ we use Schwarz's inequality again to obtain

$$|A|^2 \le \left(\sum_{kl>J} \frac{|c_{kl}|^2}{e_k e_l} \right) \left(\sum_{mn>J} e_m e_n a_m^\dagger a_n^\dagger a_m a_n \right) \tag{49}$$

for any sequence of positive numbers e_j. We choose e_j to be the eigenvalues of K_0, in which case

$$\sum_{mn>J} e_m e_n a_m^\dagger a_n^\dagger a_m a_n \le \left(\sum_{k>J} e_k a_k^\dagger a_k \right)^2 = T^2. \tag{50}$$

Moreover,

$$\sum_{kl>J} \frac{|c_{kl}|^2}{e_k e_l} = \left\langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} \left| W \left(\frac{Q}{K_0} \otimes \frac{Q}{K_0} \right) W \right| \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} \right\rangle. \tag{51}$$

We have the following two operator inequalities; the first comes from the fact that $K_0 \geq e_J$ on the range of the projector Q and the second comes from $K_0 \geq -\eta\Delta$:

$$\frac{Q}{K_0} \leq \frac{2}{K_0 + e_J} \leq \frac{2}{-\eta\Delta + e_J} \,. \tag{52}$$

Denoting the integral kernel of $(-\Delta + \mu)^{-1}$ by

$$k_\mu(x - x') = \frac{1}{4\pi} \frac{e^{-\sqrt{\mu}|x-x'|}}{|x - x'|} \,, \tag{53}$$

we see that (51) is bounded above by

$$\frac{4}{\eta^2} \int dxdydx'dy' \, \overline{\Phi_{\mathbf{z}}(x)\Phi_{\mathbf{z}}(y)} W(x - y) k_{e_J/\eta}(x - x') k_{e_J/\eta}(y - y') \Phi_{\mathbf{z}}(x')\Phi_{\mathbf{z}}(y') W(x' - y')$$

$$\leq \frac{4}{\eta^2} \int dxdydx'dy' \, |\Phi_{\mathbf{z}}(x)|^2 |\Phi_{\mathbf{z}}(y)|^2 W(x - y) k_{e_J/\eta}(x - x') k_{e_J/\eta}(y - y') W(x' - y')$$

$$\leq \frac{1}{2\pi\eta^{3/2}} \frac{\|W\|_1}{\sqrt{e_J}} I(\Phi_{\mathbf{z}}) \,. \tag{54}$$

Here, we used Young's inequality for the (x', y') integration, as well as the fact that $\|k_\mu\|_2^2 = (8\pi\sqrt{\mu})^{-1}$.

By putting all this together, we have that

$$(A + A^\dagger)^2 \leq 4\|W\|_\infty I(\Phi_{\mathbf{z}}) + \frac{32}{27\pi^4}\eta^{-1}\|W\|_1^2\|\nabla\Phi_{\mathbf{z}}\|_2^4 \, T + \frac{4}{2\pi\eta^{3/2}} \frac{\|W\|_1}{\sqrt{e_J}} I(\Phi_{\mathbf{z}}) \, T^2 \,. \tag{55}$$

Since the square root preserves operator monotonicity, we can take the square root on both sides of (55). By the triangle inequality, we can take the sum of the square roots of each term on the right side. Finally, applying the Schwarz inequality to the first and third term, we conclude that, for any $\delta > 0$,

$$|A + A^\dagger| \leq \delta I(\Phi_{\mathbf{z}}) + \frac{1}{\delta}\|W\|_\infty + \frac{4}{\pi^2}\sqrt{\frac{2}{27}}\eta^{-1/2}\|W\|_1\|\nabla\Phi_{\mathbf{z}}\|_2^2\sqrt{T}$$

$$+ e_J^{-1/4}\left(\|W\|_1 I(\Phi_{\mathbf{z}}) + \left(2\pi\eta^{3/2}\right)^{-1}\right) T \,. \tag{56}$$

We now proceed similarly with the last term in (42) which is linear in a_k and $a_k^\dagger$. Denoting $c_k = \langle \Phi_{\mathbf{z}} \otimes \Phi_{\mathbf{z}} | W | \Phi_{\mathbf{z}} \otimes \varphi_k \rangle$, we have that

$$\left(\sum_{k>J}\left(c_k a_k + \overline{c_k} a_k^\dagger\right)\right)^2 \leq 4\left(\sum_{k>J}\frac{|c_k|^2}{e_k}\right)\left(\sum_{k>J} e_k a_k^\dagger a_k\right) + 2\sum_{k>J} |c_k|^2 \,. \tag{57}$$

Using Hölder's and Sobolev's inequality,

$$\sum_{k\geq 1} |c_k|^2 = \int dxdydz \, |\Phi_{\mathbf{z}}(x)|^2 |\Phi_{\mathbf{z}}(y)|^2 |\Phi_{\mathbf{z}}(z)|^2 W(x - y) W(x - z)$$

$$\leq \|W\|_{3/2}\|\Phi_{\mathbf{z}}\|_6^2 I(\Phi_{\mathbf{z}}) \leq \frac{4}{3(2\pi^2)^{2/3}}\|W\|_\infty^{1/3}\|W\|_1^{2/3}\|\nabla\Phi_{\mathbf{z}}\|_2^2 I(\Phi_{\mathbf{z}}) \,. \tag{58}$$

Moreover, using (52) again, together with Young's and Sobolev's inequalities, as well as the fact that the $3/2$ norm of k_μ is given by $2^{-1/3}\mu^{-1/2}/3$, we find that

$$\sum_{k>J} \frac{|c_k|^2}{e_k} \leq \frac{2}{\eta} \int dx\,dy\,dx'\,dy'\, \overline{\Phi_{\mathbf{z}}(x)}|\Phi_{\mathbf{z}}(x')|^2 W(x-x')k_{e_J/\eta}(x-y)\Phi_{\mathbf{z}}(y)|\Phi_{\mathbf{z}}(y')|^2 W(y-y')$$

$$\leq \frac{2}{\eta} \int dx\,dy\,dx'\,dy'\, |\Phi_{\mathbf{z}}(x)|^2|\Phi_{\mathbf{z}}(x')|^2 W(x-x')k_{e_J/\eta}(x-y)|\Phi_{\mathbf{z}}(y')|^2 W(y-y')$$

$$\leq \frac{4}{9\pi^{4/3}}\eta^{-1/2}\frac{\|W\|_1}{\sqrt{e_J}}\|\nabla\Phi_{\mathbf{z}}\|_2^2 I(\Phi_{\mathbf{z}})\,. \tag{59}$$

This implies that

$$\left(\sum_{k>J}\left(c_k a_k + \overline{c_k}a_k^\dagger\right)\right)^2$$

$$\leq \frac{8}{3(2\pi^2)^{2/3}}\|W\|_\infty^{1/3}\|W\|_1^{2/3}\|\nabla\Phi_{\mathbf{z}}\|_2^2 I(\Phi_{\mathbf{z}}) + \frac{16}{9\pi^{4/3}}\eta^{-1/2}\frac{\|W\|_1}{\sqrt{e_J}}\|\nabla\Phi_{\mathbf{z}}\|_2^2 I(\Phi_{\mathbf{z}})\,T \tag{60}$$

$$\leq \left(\sqrt{\frac{2}{3}}\frac{1}{(2\pi^2)^{1/3}}\|W\|_\infty^{1/6}\|W\|_1^{1/3} + \frac{2}{3\pi^{2/3}}\eta^{-1/4}\|W\|_1^{1/2}e_J^{-1/4}\sqrt{T}\right)^2\left(\|\nabla\Phi_{\mathbf{z}}\|_2^2 + I(\Phi_{\mathbf{z}})\right)^2,$$

again using the triangle and the Schwarz inequality. As mentioned above, operator monotonicity is preserved by the square root, and hence we can take the square root on both sides of Eq. (60).

This completes the lower bound on the lower symbol $u(\mathbf{z})$. For the convenience of the reader, we repeat the bound just derived:

$$u(\mathbf{z}) \geq \langle\Phi_{\mathbf{z}}|K_0|\Phi_{\mathbf{z}}\rangle + I(\Phi_{\mathbf{z}})\left(1 - \delta - e_J^{-1/4}\|W\|_1 T\right) + \frac{C}{M}\left(\|\Phi_{\mathbf{z}}\|_2^2 - M\right)^2 \tag{61}$$

$$- \left(\|\nabla\Phi_{\mathbf{z}}\|_2^2 + I(\Phi_{\mathbf{z}})\right)\left(2\sqrt{\frac{2}{3}}\frac{1}{(2\pi^2)^{1/3}}\|W\|_\infty^{1/6}\|W\|_1^{1/3} + \frac{4}{3\pi^{2/3}}\eta^{-1/4}\|W\|_1^{1/2}e_J^{-1/4}\sqrt{T}\right)$$

$$- \|\nabla\Phi_{\mathbf{z}}\|_2^2\frac{4}{\pi^2}\sqrt{\frac{2}{27}}\eta^{-1/2}\|W\|_1\sqrt{T} - \frac{1}{\delta}\|W\|_\infty + T\left(1 - e_J^{-1/4}(2\pi^2\eta^{3/2})^{-1} - \frac{2C}{e_J}\right)\,.$$

We note that in the following we will choose J large enough so that the last term in (61) is positive and thus can be neglected for a lower bound. (Recall that $e_J \to \infty$ as $J \to \infty$.)

3b. Lower Bound on the Remaining Terms in $U(\mathbf{z})$.

A lower bound on the first term on the right side of (35) is given in (61) and, therefore, to get a lower bound on the upper symbol $U(\mathbf{z})$, it remains to bound the last two terms on the right side of (35). The very last term is positive, as will be shown now, and can thus be neglected for a lower bound. Namely,

$$\frac{1}{2}\left(\partial_{\mathbf{z}}\partial_{\bar{\mathbf{z}}}\right)^2 u(\mathbf{z}) = \frac{1}{2}\left(\partial_{\mathbf{z}}\partial_{\bar{\mathbf{z}}}\right)^2\left(\langle\Phi_{\mathbf{z}}\otimes\Phi_{\mathbf{z}}|W|\Phi_{\mathbf{z}}\otimes\Phi_{\mathbf{z}}\rangle + \frac{C}{M}\|\Phi_{\mathbf{z}}\|_2^4\right) \tag{62}$$

$$= \frac{1}{2}\sum_{1\leq ij\leq J}\langle\varphi_i\otimes\varphi_j + \varphi_j\otimes\varphi_i|W|\varphi_i\otimes\varphi_j + \varphi_j\otimes\varphi_i\rangle + \frac{C}{M}J(J+1) \geq 0\,.$$

The remaining expression, $\partial_{\mathbf{z}}\partial_{\bar{\mathbf{z}}}u(\mathbf{z})$, consists of the following terms. First, from the one-body part (38) of the Hamiltonian we obtain a contribution $\sum_{j\leq J}e_j$. Second, from the term (39) (see also (33)) that was introduced in order to control the particle number, we get

$$\frac{C}{M}\left\{(2N^> - 2M + 1 + 2\|\Phi_{\mathbf{z}}\|^2)J + 2\|\Phi_{\mathbf{z}}\|^2\right\} \leq \frac{2C}{M}(J+1)\|\Phi_{\mathbf{z}}\|_2^2 + \frac{JC}{M}\left(2N^> + 1\right). \quad (63)$$

Finally, the following three contributions are obtained from the interaction part. From the part where all four indices are $\leq J$, we have

$$\sum_{j\leq J}\langle\Phi_{\mathbf{z}}\otimes\varphi_j + \varphi_j\otimes\Phi_{\mathbf{z}}|W|\Phi_{\mathbf{z}}\otimes\varphi_j + \varphi_j\otimes\Phi_{\mathbf{z}}\rangle \leq 4\sum_{j\leq J}\langle\Phi_{\mathbf{z}}\otimes\varphi_j|W|\Phi_{\mathbf{z}}\otimes\varphi_j\rangle$$

$$\leq 4\sum_{j\leq J}\|W\|_1\|\Phi_{\mathbf{z}}\|_6^2\|\varphi_j\|_3^2 \;\leq\; (4/3)^{3/2}\frac{1}{2\pi^2}\eta^{-1/2}\|W\|_1\,\|\nabla\Phi_{\mathbf{z}}\|_2^2\sum_{j\leq J}\sqrt{e_j}. \quad (64)$$

Here, we used the inequalities of Young, Hölder and Sobolev as well as the facts that $-\Delta \leq \eta^{-1}K_0$ and $\langle\varphi_j|K_0|\varphi_j\rangle = e_j$ in the last step. From the term with 3 indices $\leq J$, we get

$$2\sum_{j\leq J}\sum_{k>J}\langle\Phi_{\mathbf{z}}\otimes\varphi_j + \varphi_j\otimes\Phi_{\mathbf{z}}|W|\varphi_j\otimes\varphi_k\rangle a_k + \text{adjoint}. \quad (65)$$

Using (57), this time with $e_k \equiv 1$, (65) is bounded above, as an operator, by

$$4\sum_{j\leq J}\left[\left(N^> + \tfrac{1}{2}\right)\sum_{k>J}|\langle\varphi_j\otimes\varphi_k|W|\Phi_{\mathbf{z}}\otimes\varphi_j + \varphi_j\otimes\Phi_{\mathbf{z}}\rangle|^2\right]^{1/2}. \quad (66)$$

Similarly to (58), we can derive the bound

$$\sum_{k\geq 1}|\langle\varphi_i\otimes\varphi_k|W|\Phi_{\mathbf{z}}\otimes\varphi_i + \varphi_i\otimes\Phi_{\mathbf{z}}\rangle|^2 \leq 4\|W\|_{3/2}\|W\|_1\|\Phi_{\mathbf{z}}\|_6^2\|\varphi_i\|_6^3\|\varphi_i\|_2. \quad (67)$$

Since $\|\varphi_i\|_2 = 1$ and $\|\varphi_i\|_6^2 \leq (4/3)(2\pi^2)^{-2/3}\|\nabla\varphi_i\|_2^2 \leq (4/3)(2\pi^2)^{-2/3}\eta^{-1}e_i$, this implies that

$$(66) \leq 8(4/3)^{5/4}\frac{1}{(2\pi^2)^{5/6}}\|W\|_1^{5/6}\|W\|_\infty^{1/6}\|\nabla\Phi_{\mathbf{z}}\|_2\eta^{-3/4}\sum_{i\leq J}e_i^{3/4}\sqrt{N^> + \tfrac{1}{2}}$$

$$\leq 4(4/3)^{5/4}\frac{1}{(2\pi^2)^{5/6}}\|W\|_1^{5/6}\|W\|_\infty^{1/6}\eta^{-3/4}\sum_{i\leq J}e_i^{3/4}\left(\|\nabla\Phi_{\mathbf{z}}\|_2^2 + N^> + \tfrac{1}{2}\right). \quad (68)$$

Here, Schwarz's inequality was used in the last step.

The last term to estimate is the one coming from 2 indices $\leq J$, given by

$$\sum_{j\leq J}\sum_{k,l>J}\langle\varphi_j\otimes\varphi_k + \varphi_k\otimes\varphi_j|W|\varphi_j\otimes\varphi_l + \varphi_l\otimes\varphi_j\rangle a_k^\dagger a_l$$

$$\leq (4/3)^{3/2}\frac{1}{2\pi^2}\eta^{-3/2}\|W\|_1\sum_{j\leq J}\sqrt{e_j}\,T. \quad (69)$$

This inequality can be seen as follows. For any one-particle function f,

$$\langle \varphi_i \otimes f + f \otimes \varphi_i | W | \varphi_i \otimes f + f \otimes \varphi_i \rangle \leq 4\langle \varphi_i \otimes f | W | \varphi_i \otimes f \rangle \leq 4\|W\|_1 \|f\|_6^2 \|\varphi_i\|_3^2$$

$$\leq (4/3)^{3/2} \frac{1}{2\pi^2} \eta^{-1/2} \|W\|_1 \|\nabla f\|_2^2 \sqrt{e_i} \, . \tag{70}$$

The last inequality is the same is in (64). The result now follows using $-\Delta \leq \eta^{-1} K_0$.

Altogether, we have thus shown that

$$\partial_{\mathbf{z}} \partial_{\bar{\mathbf{z}}} u(\mathbf{z}) \leq \sum_{i \leq J} e_i + \frac{2C}{M}(J+1)\|\Phi_{\mathbf{z}}\|_2^2 + \frac{2CJ}{M}\left(N^> + \tfrac{1}{2}\right)$$

$$+ (4/3)^{3/2} \frac{1}{2\pi^2} \eta^{-1/2} \|W\|_1 \left(\|\nabla\Phi_{\mathbf{z}}\|_2^2 + \eta^{-1}T\right) \sum_{i \leq J} \sqrt{e_i} \tag{71}$$

$$+ 4(4/3)^{5/4} \frac{1}{(2\pi^2)^{5/6}} \|W\|_1^{5/6} \|W\|_\infty^{1/6} \eta^{-3/4} \sum_{i \leq J} e_i^{3/4} \left(\|\nabla\Phi_{\mathbf{z}}\|_2^2 + N^> + \tfrac{1}{2}\right) \, .$$

This finishes our lower bound on the upper symbol $U(\mathbf{z})$. To summarize, we have shown the following operator lower bound to the operator $U(\mathbf{z})$:

$$U(\mathbf{z}) \geq \text{right side of (61)} \; - \; \text{right side of (71)} \, . \tag{72}$$

3c. c-Number Bound on T.

We are interested in the ground state energy of $U(\mathbf{z})$ for a fixed $\mathbf{z} \in \mathbb{C}^J$. Since T and $N^>$ are the only operators appearing in (61) and (71), this quantity can be bounded from below using (61) and (71) if we can evaluate the expectation values of T and $N^>$ in the ground state (or one of the ground states) of $U(\mathbf{z})$.

Let $\langle \cdot \rangle_{\mathbf{z}}$ denote the expectation value in a ground state of $U(\mathbf{z})$. We can use two simple facts: i.) Since $\sqrt{T}$ enters (61) negatively, we can use the concavity of the square root to replace $\langle \sqrt{T} \rangle_{\mathbf{z}}$ by $\sqrt{\langle T \rangle_{\mathbf{z}}}$ for a lower bound. ii.) Since $N^>$ appears positively in (71), and hence negatively in (72), we can replace it by the upper bound $N^> \leq T/e_J$.

For the purpose of bounding $\langle T \rangle_{\mathbf{z}}$ we can use a lower bound to $U(\mathbf{z})$ that is much simpler than (72). This is obtained by totally neglecting both the interaction part and the part controlling the particle number in $u(\mathbf{z})$. These give positive contributions to $u(\mathbf{z})$ (since $u(\mathbf{z})$ is the expectation value of $\mathcal{K}$ in the coherent state). We have to be more careful about $\partial_{\mathbf{z}} \partial_{\bar{\mathbf{z}}} u(\mathbf{z})$, however, because this contains some negative terms, as given in (71). (The annoying fact is that an upper symbol of a positive operator need not be positive, although the lower symbol is always positive.)

Proceeding in the manner just described we have that

$$U(\mathbf{z}) \geq \langle \Phi_{\mathbf{z}} | K_0 | \Phi_{\mathbf{z}} \rangle + T - \partial_{\mathbf{z}} \partial_{\bar{\mathbf{z}}} u(\mathbf{z}) \, . \tag{73}$$

Now let us estimate the various terms in $\partial_{\mathbf{z}} \partial_{\bar{\mathbf{z}}} u(\mathbf{z})$ in (71). We have $\eta\|\nabla\Phi_{\mathbf{z}}\|_2^2 \leq \langle \Phi_{\mathbf{z}} | K_0 | \Phi_{\mathbf{z}} \rangle$. Also $\|\Phi_{\mathbf{z}}\|_2^2 \leq \langle \Phi_{\mathbf{z}} | K_0 | \Phi_{\mathbf{z}} \rangle / \inf \text{spec} \left(-\eta\Delta + V(x)\right)$. Moreover, $\|W\|_1 \leq 4\pi a/N$, and $\|W\|_\infty \leq 6a/(R^3 N)$.

We will choose $R \gg N^{-2/3}$ below. Therefore, $\|W\|_\infty \ll N$. The operator $N^>$ can be bounded in terms of T as $N^> \leq T/e_J$. Note also that $M = O(N)$ by assumption. Hence we see from (71) and (73) that, for N large enough (depending on the parameters η, C and J),

$$U(\mathbf{z}) \geq \tfrac{1}{2}T - \text{const.} , \tag{74}$$

where the constant depends only on η, C and J, but not on M or N.

The value of (74) is that it allows us to control the value of $\langle T \rangle_{\mathbf{z}}$, and thereby control $\inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z})$, which is our lower bound to the ground state energy of $\mathcal{K}$. There is some number E, independent of all parameters, such that $\inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z}) \leq ME/2 - \text{const.}$ because $\inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z})$ is less than the known upper bound to the ground state energy of $\mathcal{K}$. Then we can, and will restrict our attention to $\mathbf{z}$'s with $\langle T \rangle_{\mathbf{z}} \leq ME$ because only those values of $\mathbf{z}$ are relevant for computing $\inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z})$, as (74) shows. Only the existence of E and not its value is important.

We conclude from (72) and the fact that $\langle T \rangle_{\mathbf{z}} \leq ME$ for the $\mathbf{z}$ in question that

$$\inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z}) \geq \inf_\Phi \mathcal{E}[\Phi] , \tag{75}$$

where

$$\mathcal{E}[\Phi] = \langle \Phi | K_0 | \Phi \rangle + D_1 \, I(\Phi) + \frac{C}{M} \left(\|\Phi\|_2^2 - M \right)^2 - D_2 \|\nabla\Phi\|_2^2 - D_3 - \frac{2C}{M}(J+1)\|\Phi\|_2^2 . \tag{76}$$

The notation is the following:

$$D_1 = 1 - \delta - e_J^{-1/4}\|W\|_1 ME - 2\sqrt{\frac{2}{3}}\frac{1}{(2\pi^2)^{1/3}}\|W\|_\infty^{1/6}\|W\|_1^{1/3}$$
$$- \frac{4}{3\pi^{2/3}}\eta^{-1/4}\|W\|_1^{1/2}e_J^{-1/4}M^{1/2}E^{1/2} , \tag{77}$$

$$D_2 = 2\sqrt{\frac{2}{3}}\frac{1}{(2\pi^2)^{1/3}}\|W\|_\infty^{1/6}\|W\|_1^{1/3} + \frac{4}{3\pi^{2/3}}\eta^{-1/4}\|W\|_1^{1/2}e_J^{-1/4}M^{1/2}E^{1/2}$$
$$+ \frac{4}{\pi^2}\sqrt{\frac{2}{27}}\eta^{-1/2}\|W\|_1 M^{1/2}E^{1/2} + (4/3)^{3/2}\frac{1}{2\pi^2}\eta^{-1/2}\|W\|_1 \sum_{i \leq J}\sqrt{e_i}$$
$$+ 4(4/3)^{5/4}\frac{1}{(2\pi^2)^{5/6}}\|W\|_1^{5/6}\|W\|_\infty^{1/6}\eta^{-3/4}\sum_{i \leq J}e_i^{3/4} , \tag{78}$$

and

$$D_3 = \sum_{i \leq J}e_i + \frac{2CJ}{M}\left(ME/e_J + \tfrac{1}{2}\right) + (4/3)^{3/2}\frac{1}{2\pi^2}\eta^{-3/2}\|W\|_1 ME \sum_{i \leq J}\sqrt{e_i}$$
$$+ 4(4/3)^{5/4}\frac{1}{(2\pi^2)^{5/6}}\|W\|_1^{5/6}\|W\|_\infty^{1/6}\eta^{-3/4}\sum_{i \leq J}e_i^{3/4}\left(MEe_J^{-1} + \tfrac{1}{2}\right) + \frac{1}{\delta}\|W\|_\infty . \tag{79}$$

We have neglected the last term in (61) containing $(1 - e_J^{-1/4}(2\pi^2\eta^{3/2})^{-1} - 2C/e_J)$, assuming J to be large enough to make this term positive. (Recall that $e_J \to \infty$ as $J \to \infty$.)

Our final result in this section, (75)–(76), might not appear to be useful at first sight, but the reader should note that the first two terms in (76) are essentially the GP energy expression. The term $\langle \Phi | K_0 | \Phi \rangle$ is the relevant (i.e., low momentum) part of the kinetic energy $\int |(i\nabla - A)\Phi|^2$. The coefficient D_1 equals 1 to leading order and $I(\Phi)$ is essentially the GP quartic term $4\pi a \int |\Phi|^4$ (up to errors which will be controlled). Moreover, for C large enough the term $C(\|\Phi\|_2^2 - M)^2/M$ ensures that we have the right particle number. For an appropriate choice of the parameters J, η and R all other terms are of lower order as $N \to \infty$, as we shall show.

STEP 4. Bounds on Three-Particle Density.

So far we have bounded the main term in (26), namely $\inf \operatorname{spec} K$. Of the various other terms in (26) that have to be bounded, the one that is most intuitively negligible, but which we find the hardest to control is the last term in (26). To show that it is small we have to show that the probability of finding three particles within a distance $2R$ of each other (in a true ground state of $H_{M,N}$) is small. This is accomplished in this section.

We begin with a lemma about the possible size of the expectation value of a function of the coordinates of three bosons. Recall from Step 2 that $\langle \, \cdot \, \rangle_{\mathcal{B}}$ denotes expectation value in the *bosonic*, zero-temperature state of the M-body Hamiltonian $H_{M,N}$.

Lemma 2. *Let $\xi(x_1, x_2, x_3)$ be any positive function of x_1, x_2 and $x_3 \in \mathbb{R}^3$. With $V =$ the one-body potential appearing in $H_{M,N}$, we define the three-body, independent particle Hamiltonian*

$$h = -\Delta_1 - \Delta_2 - \Delta_3 + V(x_1) + V(x_2) + V(x_3) \ .$$

Let $\alpha > 0$ and let $e^{-\alpha h}(x_1, x_2, x_3 \; ; \; y_1, y_2, y_3)$ be the 'heat kernel' of h at 'inverse temperature' α. Finally, consider the modified integral kernel

$$e^{-\alpha h}(x_1, x_2, x_3 \; ; \; y_1, y_2, y_3)\sqrt{\xi(x_1, x_2, x_3)\xi(y_1, y_2, y_3)} \tag{80}$$

and let Λ denote its largest eigenvalue (i.e., its norm as a map from $L^2(\mathbb{R}^9)$ to $L^2(\mathbb{R}^9)$). Then

$$\left\langle \xi(x_1, x_2, x_3) \right\rangle_{\mathcal{B}} \le \Lambda \exp\{\alpha(E_0(M, N) - E_0(M - 3, N))\} \ . \tag{81}$$

Note that for the M and N under consideration here, we have $E_0(M, N) - E_0(M-3, N) \le 3Z$, as explained in Step 1. It is the appearance of the peculiar difference $E_0(M, N) - E_0(M-3, N)$ in Lemma 2 that led us to the discussion in Step 1. If the three-body correlations could be bounded more expeditiously than is done here, Step 1 could be simplified.

Proof. We denote by $\operatorname{Tr}[\cdot]$ the trace over *all* of $L^2(\mathbb{R}^{3M})$, not just the bosonic states, and by P_{b} the projection onto the bosonic (i.e., symmetric) subspace. Note that $\exp\{-\beta H_{M,N}\}$ is trace class for large enough β, by our assumption on the logarithmic increase of the potential $V(x)$. (This follows from the Feynman-Kac-Itô formula, together with the results in the appendix.) Hence

$$\langle \xi \rangle_{\mathcal{B}} = \lim_{n \to \infty} \frac{\operatorname{Tr}\left[\xi e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]}{\operatorname{Tr}\left[e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]} \ , \tag{82}$$

independently of α, of course. Note that $H_{M,N}$ commutes with P_{b} so $e^{-\alpha n H_{M,N}} P_{\mathrm{b}}$ is self-adjoint and positive. The multiplication operator ξ is also positive and we can write $\xi e^{-\alpha n H_{M,N}} P_{\mathrm{b}} = [\xi e^{-\alpha H_{M,N}} P_{\mathrm{b}}] e^{-\alpha(n-1)H_{M,N}} P_{\mathrm{b}}$. Hölder's inequality for traces of positive operators states that $\mathrm{Tr} AB \leq \{\mathrm{Tr} A^n\}^{1/n} \{\mathrm{Tr} B^{n/(n-1)}\}^{(n-1)/n}$, and therefore

$$\frac{\mathrm{Tr}\left[\xi e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]}{\mathrm{Tr}\left[e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]} \leq \left(\frac{\mathrm{Tr}\left[(\xi e^{-\alpha H_{M,N}} P_{\mathrm{b}})^n\right]}{\mathrm{Tr}\left[e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]}\right)^{1/n}. \tag{83}$$

Consider the bigger projection $\widehat{P_{\mathrm{b}}}$, which symmetrizes only among particles $4, 5, \ldots, M$. It commutes with $H_{M,N}$ and also with ξ, and hence $e^{-\alpha H_{M,N}} P_{\mathrm{b}} \leq e^{-\alpha H_{M,N}} \widehat{P_{\mathrm{b}}}$. Since $\xi \geq 0$, this yields the upper bound

$$\left(\frac{\mathrm{Tr}\left[(\xi e^{-\alpha H_{M,N}} P_{\mathrm{b}})^n\right]}{\mathrm{Tr}\left[e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]}\right)^{1/n} \leq \left(\frac{\mathrm{Tr}\left[\widehat{P_{\mathrm{b}}}(\xi e^{-\alpha H_{M,N}})^n\right]}{\mathrm{Tr}\left[e^{-\alpha n H_{M,N}} P_{\mathrm{b}}\right]}\right)^{1/n}. \tag{84}$$

We now claim that

$$\mathrm{Tr}\left[\widehat{P_{\mathrm{b}}}(\xi e^{-\alpha H_{M,N}})^n\right] \leq \mathrm{Tr}_3\,(\xi e^{-\alpha h})^n\,\mathrm{Tr}_{M-3}\left[e^{-\alpha n H_{M-3,N}}\widehat{P_{\mathrm{b}}}\right], \tag{85}$$

where Tr_3 and Tr_{M-3} denote the trace over the first 3 and last $M-3$ particles, respectively. Taking the limit $n \to \infty$ this proves (81).

To show (85), we write $H_{M,N} = H_{3,N} \otimes \mathbb{I}_{M-3} + \mathbb{I}_3 \otimes H_{M-3,N} + W$, with W denoting the interaction between the first 3 and the last $M-3$ particles. Note that $W \geq 0$. Using the Trotter product formula, we first replace each factor $e^{-\alpha H_{M,N}}$ by $(e^{-\alpha H_{3,N}/m} e^{-\alpha(H_{M-3,N}+W)/m})^m$ for some integer m. (Here we abuse the notation slightly, omitting to write tensor products and identity operators.) For $\mathbf{x} = (x_1, x_2, x_3)$, let $k(\mathbf{x}, \mathbf{x}')$ denote the integral kernel of $e^{-\alpha H_{3,N}/m}$. Denoting by $W_{\mathbf{x}}$ the multiplication operator on the subspace of the last $M-3$ particles obtained by fixing the first 3 to have positions $\mathbf{x}$, and introducing nm integration variables $\mathbf{x}_{ij}$, $1 \leq i \leq n$, $1 \leq j \leq m$, we can write

$$\mathrm{Tr}\left[\widehat{P_{\mathrm{b}}}\left(\xi\left(e^{-\alpha H_{3,N}/m} e^{-\alpha(H_{M-3,N}+W)/m}\right)^m\right)^n\right] =$$
$$\int \prod_{ij} d\mathbf{x}_{ij} \prod_i \xi(\mathbf{x}_{i1}) \prod_{ij} k(\mathbf{x}_{ij}, \mathbf{x}_{i(j+1)}) \,\mathrm{Tr}_{M-3}\left[\widehat{P_{\mathrm{b}}} \prod_{i,j} e^{-\alpha(H_{M-3,N}+W_{\mathbf{x}_{ij}})/m}\right], \tag{86}$$

where we identify $\mathbf{x}_{i(m+1)} \equiv \mathbf{x}_{(i+1)1}$ and $\mathbf{x}_{n(m+1)} \equiv \mathbf{x}_{1,1}$. By Hölder's inequality for traces, we can estimate

$$\left|\mathrm{Tr}_{M-3}\left[\widehat{P_{\mathrm{b}}} \prod_{i,j} e^{-\alpha(H_{M-3,N}+W_{\mathbf{x}_{ij}})/m}\right]\right| \leq \sup_{ij} \mathrm{Tr}_{M-3}\left[\widehat{P_{\mathrm{b}}} e^{-\alpha n(H_{M-3,N}+W_{\mathbf{x}_{ij}})}\right]$$
$$\leq \mathrm{Tr}_{M-3}\left[\widehat{P_{\mathrm{b}}} e^{-\alpha n H_{M-3,N}}\right], \tag{87}$$

where in the last inequality we used the fact that $W_{\mathbf{x}} \geq 0$ and that the partition function is monotone in the potential. By the Feynman-Kac-Itô formula [24, Sect. 15], the integral

kernel $k(\mathbf{x}, \mathbf{x}')$ is bounded in absolute value by the kernel of $e^{-\alpha h/m}$. Using this estimate and rewriting the integrals as a trace we obtain

$$\text{Tr}\left[\widehat{P_{\text{b}}}\left(\xi\left(e^{-\alpha H_{3,N}/m}e^{-\alpha(H_{M-3,N}+W)/m}\right)^m\right)^n\right] \leq \text{Tr}_3\left(\xi e^{-\alpha h}\right)^n \text{Tr}_{M-3}\left[e^{-\alpha n H_{M-3,N}}\widehat{P_{\text{b}}}\right]. \tag{88}$$

Letting $m \to \infty$ this yields (85). $\qquad\square$

We now use Lemma 2 to obtain a bound on the various terms in (26) and (27). Lemma 2 immediately implies that

$$\left\langle |x_1|^2 \right\rangle_{\mathcal{B}} \leq e^{3\alpha Z} \||x|e^{\alpha(\Delta-V(x))}|x|\|_{\infty}, \tag{89}$$

with $\|\cdot\|_{\infty}$ denoting operator norm. For positive operators, the operator norm is bounded by the trace, in this case given by $\text{Tr}|x|^2 e^{\alpha(\Delta-V(x))}$. This expression, in turn, is bounded for α large enough, as shown in the appendix. In exactly the same way we can bound $\langle |x_1|^4 \rangle_{\mathcal{B}}$.

Moreover, we have that

$$\left\langle w_R(x_1 - x_2) \right\rangle_{\mathcal{B}} \leq e^{3\alpha Z} \|\sqrt{w_R} e^{-\alpha h} \sqrt{w_R}\|_{\infty} \leq e^{3\alpha Z} \frac{1}{(4\pi\alpha)^{3/2}} \int_{\mathbb{R}^3} w_R(x) dx. \tag{90}$$

The last inequality can be seen as follows. Denote by $k(x, x')$ the kernel of $e^{\alpha(\Delta-V(x))}$. The Feynman-Kac formula implies that $k(x, x') \leq (4\pi\alpha)^{-3/2}$ for any positive $V(x)$. Hence, for any function $f \in L^2(\mathbb{R}^6)$,

$$\int dx dx' dy dy' \overline{f(x,y)} \sqrt{w_R(x-y)} k(x,x') k(y,y') \sqrt{w_R(x'-y')} f(x,y)$$

$$\leq (4\pi\alpha)^{-3/2} \int dx dx' k(x,x') \left[\int dy \sqrt{w_R(x-y)}|f(x,y)|\right]\left[\int dy \sqrt{w_R(x'-y)}|f(x',y)|\right]$$

$$\leq (4\pi\alpha)^{-3/2}\left(\int w_R\right)\int dx dx' k(x,x')\left[\int dy|f(x,y)|^2\right]^{1/2}\left[\int dy|f(x',y)|^2\right]^{1/2}, \tag{91}$$

where we used Schwarz's inequality in the last step. The result now follows from the fact that $e^{\alpha(\Delta-V(x))} \leq \mathbb{I}$.

Similarly, repeating the above argument with x_2 in place of x and (x_1, x_3) in place of y, we obtain

$$\left\langle U_R(x_1 - x_2)\theta(2R - |x_2 - x_3|) \right\rangle_{\mathcal{B}} \leq e^{3\alpha Z} \frac{1}{(4\pi\alpha)^3} \int_{\mathbb{R}^3} U_R(x) dx \int_{\mathbb{R}^3} \theta(2R - |x|) dx$$

$$= e^{3\alpha Z} \frac{1}{\alpha^3} \frac{2}{3\pi} R^3. \tag{92}$$

This finishes our bounds on the various terms appearing in (26) and (27).

STEP 5. Collection of All the Terms and the Final Inequality.

In this section we concatenate the various pieces of the lower bound to the energy $E_0(M, N)$ in (26), and finish the proof of Proposition 1. Inequality (26) contains several terms. All

except $\inf \operatorname{spec} K$ were bounded in Step 4 and in (27). The essence of Step 3 is the bound on the main term

$$\inf \operatorname{spec} K \geq \inf_{\mathbf{z}} \inf \operatorname{spec} U(\mathbf{z}) \geq \inf_{\Phi} \mathcal{E}[\Phi] \,, \tag{93}$$

where $\mathcal{E}[\Phi]$ is defined in (76).

Let us begin by disposing of the terms mentioned in Step 4. As shown there, $\langle |x_1|^2 \rangle_{\mathcal{B}} \leq$ const. and $\langle |x_1|^4 \rangle_{\mathcal{B}} \leq$ const. for some constant depending only on Z. (Recall that Z is a fixed number of order 1.) Moreover, from (90) and (29) we see that (recalling that $M \leq N$)

$$\frac{M^2 a}{N^2 \varepsilon} \langle w_R(x_1 - x_2) \rangle_{\mathcal{B}} \leq \text{const.} \frac{a}{\varepsilon} \frac{R^2}{s^2} \,. \tag{94}$$

This term will thus be negligible, if $R \to 0$ as $N \to \infty$ (keeping ε and s fixed for the moment). We are free to choose the dependence of R on N, and we choose R to satisfy

$$N^{-1/3} \gg R \gg N^{-2/3} \quad \text{as} \quad N \to \infty \,. \tag{95}$$

The last term to estimate is then

$$\frac{aM^3}{N^2} \langle U_R(x_1 - x_2)\theta(2R - |x_2 - x_3|) \rangle_{\mathcal{B}} \leq \text{const.} \, aNR^3 \ll 1 \,. \tag{96}$$

Hence it follows from (26) and (27) that, for any fixed s, ε and η (recalling that $\lambda = \lim_{N\to\infty} M/N$),

$$\lim_{N\to\infty} \frac{1}{N}(1 + 4\eta)E_0(M, N) \geq \lim_{N\to\infty} \frac{1}{N} \inf_{\Phi} \mathcal{E}[\Phi] + \lambda \kappa(\eta) - \text{const.} \, \lambda \eta \,. \tag{97}$$

The only thing left is the minimization of $\mathcal{E}[\Phi]$ given in (76), which contains the numbers D_1, D_2 and D_3 in (77)–(79). To evaluate them as $N \to \infty$ we note that $\|W\|_1 \leq 4\pi a/N$, and $\|W\|_\infty \ll N$ for our choice of R in (95). Hence, we see that

$$\lim_{\delta\to 0} \lim_{J\to\infty} \lim_{N\to\infty} D_1 = 1 \,, \quad \lim_{J\to\infty} \lim_{N\to\infty} D_2 = 0 \,, \quad \text{and} \quad \lim_{N\to\infty} \frac{1}{N}D_3 = 0 \,. \tag{98}$$

Using the fact that both $\|\nabla\Phi\|_2^2$ and $\|\Phi\|_2^2$ are bounded relative to $\langle \Phi|K_0|\Phi \rangle$, and rescaling $\Phi \to M^{1/2}\Phi$, we obtain

$$\lim_{J\to\infty} \lim_{N\to\infty} \frac{1}{N} \inf_{\Phi} \mathcal{E}[\Phi] \geq \tag{99}$$

$$\lim_{R\to 0} \inf_{\Phi} \left\{ \lambda\langle\Phi|K_0|\Phi\rangle + (1 - \varepsilon)a\lambda^2 \int |\Phi(x)|^2|\Phi(y)|^2 U_R(x - y)dxdy + C\lambda \left(\|\Phi\|_2^2 - 1 \right)^2 \right\} \,.$$

Note that the infimum can obviously be restricted to a set of bounded $\langle\Phi|K_0|\Phi\rangle$, independent of R, since $U_R \geq 0$. Since $K_0 \geq -\eta\Delta$ this implies that we can assume that $\|\nabla\Phi\|_2$ is bounded independent of R, and hence also $\|\Phi\|_6$ by Sobolev's inequality. Using the inequality (proved below)

$$\left| \int |\Phi(x)|^2|\Phi(y)|^2 U_R(x - y)dxdy - 4\pi\|\Phi\|_4^4 \right| \leq 8\pi R\|\Phi\|_6^3\|\nabla\Phi\|_2 \,, \tag{100}$$

we see that we can interchange the limit and the infimum and thus obtain

$$\varliminf_{J\to\infty}\lim_{N\to\infty}\frac{1}{N}\inf_{\Phi}\mathcal{E}[\Phi]\geq\inf_{\Phi}\left\{\lambda\langle\Phi|K_0|\Phi\rangle+(1-\varepsilon)4\pi a\lambda^2\|\Phi\|_4^2+C\lambda\left(\|\Phi\|_2^2-1\right)^2\right\}. \quad (101)$$

Ineq. (100) can be obtained in the following way. Using Schwarz's inequality, as well as $\int U_R(y)dy=4\pi$,

$$\left|\int|\Phi(x)|^2|\Phi(y)|^2U_R(x-y)dxdy-4\pi\|\Phi\|_4^4\right|$$

$$\leq\int dyU_R(y)\int dx|\Phi(x)|^2\left(|\Phi(x)|+|\Phi(x+y)|\right)||\Phi(x)|-|\Phi(x+y)||$$

$$\leq 2\|\Phi\|_6^3\int dyU_R(y)\left(\int dx\,||\Phi(x)|-|\Phi(x+y)||^2\right)^{1/2}. \quad (102)$$

The result now follows from the fact that $\||\Phi|-|\Phi(\,\cdot\,+y)|\|_2\leq|y|\|\nabla\Phi\|_2$, which can be seen by evaluating the norm in Fourier space, using $|1-e^{-ip\cdot y}|^2\leq|y|^2|p|^2$, and also using the fact that $\int U_R(y)|y|dy\leq R\int U_R(y)dy=4\pi R$.

Now, letting $C\to\infty$, we infer from (101) that

$$\lim_{C\to\infty}\varliminf_{J\to\infty}\lim_{N\to\infty}\frac{1}{N}\inf_{\Phi}\mathcal{E}[\Phi]\geq\inf_{\|\Phi\|_2=1}\left\{\lambda\langle\Phi|K_0|\Phi\rangle+(1-\varepsilon)4\pi a\lambda^2\|\Phi\|_4^2\right\}. \quad (103)$$

The final step is to remove the momentum cutoff in K_0, i.e., to let $s\to 0$ in Eq. (103). Again, we claim that we can interchange the limit and the infimum, at least to obtain a lower bound. Let Φ_s denote a minimizer of the functional on the right side of (103). Since $K_0\geq-\eta\Delta+V(x)$ and $V(x)\to\infty$ as $|x|\to\infty$, a sequence Φ_{s_j} with $s_j\to 0$ as $j\to\infty$ lies in a compact subset of $L^2(\mathbb{R}^3)$, and hence there exists a subsequence which converges strongly and pointwise almost everywhere [11] (both in p-space and x-space) to a function Φ_0 as $j\to\infty$, with $\|\Phi_0\|_2=1$. All the s-independent terms in the functional on the right side of (103) are weakly lower semicontinuous. Moreover, by Fatou's Lemma [11],

$$\lim_{s\to 0}\int p^2\left(1-\chi_s(p)^2\right)|\widehat{\Phi}_s(p)|^2dp\geq\int p^2|\widehat{\Phi}_0(p)|^2dp. \quad (104)$$

Hence the infimum and the limit $s\to 0$ can be interchanged for a lower bound. In combination with inequalities (103) and (97), we find that

$$\lim_{N\to\infty}\frac{1}{N}(1+4\eta)E_0(M,N)$$

$$\geq\inf_{\|\Phi\|_2=1}\left\{\lambda\left\langle\Phi\left|-\Delta+2p\cdot A(x)+A(x)^2+V(x)\right|\Phi\right\rangle+(1-\varepsilon)4\pi a\lambda^2\|\Phi\|_4^2\right\}-\text{const.}\,\lambda\eta. \quad (105)$$

(For a lower bound we simply dropped the positive terms $-2\eta\Delta$ and $\eta|x|^4$ in K_0.) By letting $\eta\to 0$ and $\varepsilon\to 0$ Proposition 1 is proved. As explained in Step 1, this proves Theorem 1.

Remark about the optimal choice of the parameters: In Eq. (95) we showed how the parameter R has to depend on N, as $N\to\infty$, in order to obtain the correct limit for the energy. The explicit dependence on N of the other parameters J, C, s, η and ε need not be specified so closely (unless we wish to obtain a detailed error estimate). It suffices to let $J\to\infty$, $C\to\infty$, $s\to 0$, $\eta\to 0$ and $\varepsilon\to 0$ (in this order) after taking the $N\to\infty$ limit.

3   Proof of Theorem 2

STEP 1. Proof of Part (i).

The fact that Γ is a convex set follows easily from its definition. Namely, if γ_N and $\bar{\gamma}_N$ are two approximate ground state sequences, and $0 \leq \lambda \leq 1$, then $\lambda\gamma_N + (1-\lambda)\bar{\gamma}_N$ is certainly also an approximate ground state sequence, whose reduced one particle density matrix is given by $\lambda\gamma_N^{(1)} + (1-\lambda)\bar{\gamma}_N^{(1)}$.

Compactness of Γ is also not difficult to see. Given a sequence $\gamma_i \in \Gamma$, the Banach-Alaoglu Theorem implies the existence of a subsequence such that $\gamma_i \rightharpoonup \gamma_\infty$ for some γ_∞ in the weak-* sense as $i \to \infty$. As already remarked in the introduction, the fact that $\mathrm{Tr}\, H_0\gamma_i \leq$ const. implies that $\gamma_i \to \gamma_\infty$ in trace norm. To prove compactness we have to show that $\gamma_\infty \in \Gamma$.

By definition, corresponding to every γ_i there is an approximate ground state sequence $\gamma_{N,i}$. That is, there is a number N_i such that $N \geq N_i$ implies that $\|\gamma_{N,i}^{(1)} - \gamma_i\| \leq 1/i$ and $|N^{-1}\mathrm{Tr}\, H_N\gamma_{N,i} - E^{\mathrm{GP}}(a)| \leq 1/i$. (Here, $\|\cdot\|$ denotes trace norm.) We can assume that $N_i \to \infty$ as $i \to \infty$. Now, for given N, let $\hat{i}(N)$ be the largest integer i such that $N \geq N_i$. Then $\hat{i}(N) \to \infty$ as $N \to \infty$, and hence the sequence $\gamma_{N,\hat{i}(N)}$ is an approximate ground state sequence. Moreover, $\|\gamma_{N,\hat{i}(N)}^{(1)} - \gamma_\infty\| \leq \|\gamma_{N,\hat{i}(N)}^{(1)} - \gamma_{\hat{i}(N)}\| + \|\gamma_{\hat{i}(N)} - \gamma_\infty\| \to 0$ as $N \to \infty$. This proves that $\gamma_\infty \in \Gamma$, and hence Γ is compact.

STEP 2. An Extension of Theorem 1.

A key step in the proof of Theorem 2 is an extension of the lower bound in Theorem 1 to the case of a perturbed Hamiltonian, where we replace the one-particle part H_0 of the Hamiltonian (1) by $H_0 + S$, where S is a bounded hermitian operator on the one-particle space $L^2(\mathbb{R}^3)$. Let $H_N^{(S)}$ denote the perturbed N-particle operator

$$H_N^{(S)} = H_N + \sum_{i=1}^{N} S^{(i)},$$

and let $E_0^{(S)}(N) = \inf\mathrm{spec}\, H_N^{(S)}$ denote its ground state energy. Correspondingly, define the perturbed GP functional $\mathcal{E}_{(S)}^{\mathrm{GP}}$ as in (5), with $H_0 + S$ in place of H_0, and let $E_{(S)}^{\mathrm{GP}}(a)$ denote its infimum over all ϕ with $\|\phi\|_2 = 1$. Then we have the following extension of Theorem 1, to whose proof we will devote the remainder of this subsection.

Proposition 2. *For all bounded hermitian operators S,*

$$\liminf_{N\to\infty} \frac{1}{N} E_0^{(S)}(N) \geq E_{(S)}^{\mathrm{GP}}(a). \tag{106}$$

We start by noting that in order to prove Proposition 2 it suffices to prove it in the special case in which S is a finite rank operator with exponentially decaying eigenfunctions. In particular, we can assume that its integral kernel $S(x,y)$ satisfies a bound

$$|S(x,y)| \leq B\exp\left(-D(|x| + |y|)\right) \tag{107}$$

for some positive constants B and D. This can be seen as follows. Let $\{f_i\}_{i=1}^\infty$ be an orthonormal basis for $L^2(\mathbb{R}^3)$ such that $|f_i(x)| < B_i \exp(-D_i|x|)$ for some choice of constants B_i, $D_i > 0$ and let P_n denote the projection onto the first n of these functions. Clearly, $P_n \to \mathbb{I}$ strongly as $n \to \infty$. Then, for any bounded S, $P_n S P_n$ is of the desired form, i.e., it has finite rank and its integral kernel satisfies a bound of the form (107). For any one-particle density matrix γ,

$$\left| \text{Tr}\big[\gamma(S - P_n S P_n)\big] \right| \leq \left\| \frac{1}{\sqrt{H_0}}\big(S - P_n S P_n\big)\frac{1}{\sqrt{H_0}} \right\| \text{Tr}[H_0\gamma] , \tag{108}$$

with $\| \cdot \|$ denoting operator norm. Since $H_0^{-1/2}$ is compact and, therefore, is the norm limit of finite rank operators, it is easy to see that the norm in (108) goes to zero as $n \to \infty$. On the other hand the set of numbers $\text{Tr}[H_0\gamma]$ that arise from those γ's that come from approximate ground states is bounded. Consequently, both sides of (106) can be approximated to within any desired ε by replacing S by $P_n S P_n$ and choosing n large enough — which implies the statement.

Thus we can assume (107) henceforth. The proof of Proposition 2 then follows exactly the same lines as the proof of Theorem 1. In fact, our proof of Theorem 1 has the advantage of being almost completely independent of the exact form of the Hamiltonian. The only place where we used the explicit form is Lemma 2, which was used to bound expectation values of certain one-, two- and three-body operators in the zero-temperature state of $H_{M,N}$. We now have to bound the expectation value of these operators in the zero-temperature state of $H_{M,N}^{(S)}$, which we denote as $\langle \cdot \rangle_\mathcal{B}^{(S)}$. (Here, the operator $H_{M,N}^{(S)}$ is defined in the obvious way. Its ground state energy will be denoted by $E_0^{(S)}(M,N)$.) To this end, Lemma 2 can be extended in the following way.

Lemma 3. *Let $\xi(x_1, x_2, x_3)$ be any positive function of x_1, x_2 and $x_3 \in \mathbb{R}^3$. Let $\widehat{S}$ denote the rank one operator on the one-particle space with integral kernel given by the right side of (107). With $V =$ the one-body potential appearing in $H_{M,N}$, we define the three-body, independent particle Hamiltonian*

$$h^{(S)} = -\Delta_1 - \Delta_2 - \Delta_3 + V(x_1) + V(x_2) + V(x_3) - \widehat{S}_1 - \widehat{S}_2 - \widehat{S}_3 . \tag{109}$$

Let $\alpha > 0$ and let $e^{-\alpha h^{(S)}}(x_1, x_2, x_3 ; y_1, y_2, y_3)$ be the 'heat kernel' of $h^{(S)}$ at 'inverse temperature' α. Finally, consider the modified integral kernel

$$e^{-\alpha h^{(S)}}(x_1, x_2, x_3 ; y_1, y_2, y_3)\sqrt{\xi(x_1, x_2, x_3)\xi(y_1, y_2, y_3)} \tag{110}$$

and let $\Lambda^{(S)}$ denote its largest eigenvalue (i.e., its norm as a map from $L^2(\mathbb{R}^9)$ to $L^2(\mathbb{R}^9)$). Then

$$\big\langle \xi(x_1, x_2, x_3)\big\rangle_\mathcal{B}^{(S)} \leq \Lambda^{(S)} \exp\{\alpha(E_0^{(S)}(M,N) - E_0^{(S)}(M-3,N))\} . \tag{111}$$

The proof follows along the same lines as the proof of Lemma 2, except for one step. Before Eq. (88), it was necessary to get an upper bound on the absolute value of the integral kernel of $\exp\{-\alpha H_{3,N}/m\}$ in terms of the kernel of $\exp\{-\alpha h/m\}$, which can be obtained

with the help of the Feynman-Kac-Itô formula. In the case considered here, we need an upper bound on the integral kernel of $\exp\{-\alpha H_{3,N}^{(S)}/m\}$. We will now show that the absolute value of this kernel is bounded above by the kernel of $\exp\{-\alpha h^{(S)}/m\}$ for the modified three-particle operator $h^{(S)}$ in (109).

This claim follows from the Trotter product formula, together with the Feynman-Kac-Itô formula, in the following way. Since S is a bounded (in fact, finite rank) operator, we can write

$$e^{-\alpha H_{3,N}^{(S)}/m} = \lim_{n \to \infty} \left[e^{-\alpha H_{3,N}/n} \left(1 - \frac{\alpha}{n} S \right) \right]^{n/m}. \tag{112}$$

By the Feynman-Kac-Itô formula, (107) and the definition of $\widehat{S}$,

$$\left| \left[e^{-\alpha H_{3,N}/n} \left(1 - \frac{\alpha}{n} S \right) \right]^{n/m} (x, y) \right| \leq \left[e^{-\alpha h/n} \left(1 + \frac{\alpha}{n} \widehat{S} \right) \right]^{n/m} (x, y). \tag{113}$$

In the limit $n \to \infty$, the operator on the right side converges strongly to $e^{-\alpha h^{(S)}/m}$. This proves our claim.

For the application of this Lemma, as in Section 2, Step 4, it is necessary to have some bounds on the kernel of $e^{-\alpha h^{(S)}}$. In particular, we need that the kernel is bounded, and that its diagonal decays for large $|x|$ at least like $|x|^{-\text{const.} \alpha}$ for some positive constant. As for the case $S = 0$, these properties are again shown in the appendix. It is there that the exponential decay of the kernel of $\widehat{S}$ gets used.

As already mentioned, except for the replacement of Lemma 2 by Lemma 3, the proof of Proposition 2 consists of simply mimicking the discussion of the proof of Theorem 1 given in Section 2.

STEP 3. Γ Contains Projections onto GP Minimizers.

Let $\Phi^{\text{GP}} \subset L^2(\mathbb{R}^3)$ denote the *set* of all minimizers of the GP functional (5). We now consider the special case where $S = -|\phi\rangle\langle\phi|$ for some $\phi \in \Phi^{\text{GP}}$. In this case, we claim that

$$\lim_{N \to \infty} \frac{1}{N} E_0^{(\lambda S)}(N) = E^{\text{GP}}(a) - \lambda \tag{114}$$

for any $\lambda \geq 0$. Given Theorem 1, the lower bound is trivial in this case. The upper bound can be derived in the same way as the upper bound for Theorem 1 in [23]. The arguments there also apply to this case, and the expectation value of S in the trial state can easily be estimated using the methods in [5, 15]. (In the non-rotating case, this was carried out in [21].)

Taking the derivative of (114) at $\lambda > 0$, Griffiths' argument [9, 18] implies that the one-particle density matrix of a ground state of $H_N^{(\lambda S)}$ converges to $|\phi\rangle\langle\phi|$ as $N \to \infty$ in this case. Hence, by a similar 'diagonal' argument as at the end of the proof of part (i) of Theorem 2, we can find a sequence λ_N with $\lambda_N \to 0$ as $N \to \infty$ such that the ground state of $H_N^{(\lambda_N S)}$ represents an approximate ground state sequence for the $\lambda = 0$ problem, and its reduced one-particle density matrix converges to $|\phi\rangle\langle\phi|$ as $N \to \infty$. This shows that $|\phi\rangle\langle\phi| \in \Gamma$ for any $\phi \in \Phi^{\text{GP}}$.

(Remark: The claim of this subsection can in principle be proved by simply constructing an appropriate approximate ground state. However, although the one-particle density matrix of the trial state used in [23] converges to $|\phi\rangle\langle\phi|$ as $N \to \infty$, this does not immediately imply that $|\phi\rangle\langle\phi| \in \Gamma$ since the trial state is not symmetric! This explains the somewhat different reasoning in this subsection.)

We note that also $|\phi\rangle\langle\phi| \in \Gamma_{\text{ext}}$ for all $\phi \in \Phi^{\text{GP}}$. This follows from the fact that all elements of Γ are positive operators, and a rank one operator cannot be written as a non-trivial convex combination of two positive operators. In the next subsection, we will show that all elements of Γ_{ext} are of the form $|\phi\rangle\langle\phi|$ with $\phi \in \Phi^{\text{GP}}$.

STEP 4. Proof of Parts (ii) and (iii).

For a given $\gamma \in \Gamma$, let γ_N be an approximate ground state sequence for H_N, with $\gamma_N^{(1)} \to \gamma$ as $N \to \infty$. By Proposition 2 we have that, for any bounded hermitian operator S and any $\lambda \in \mathbb{R}$,

$$E^{\text{GP}}(a) + \lambda \operatorname{Tr} S\gamma = \lim_{N\to\infty} \frac{1}{N} \operatorname{Tr} H_N^{(\lambda S)} \gamma_N \geq E_{(\lambda S)}^{\text{GP}}(a). \tag{115}$$

Upon dividing by λ and letting $\lambda \to 0$, this yields

$$\operatorname{Tr} S\gamma \geq \lim_{\lambda \searrow 0} \frac{E_{(\lambda S)}^{\text{GP}}(a) - E^{\text{GP}}(a)}{\lambda}. \tag{116}$$

We claim that

$$\lim_{\lambda \searrow 0} \frac{E_{(\lambda S)}^{\text{GP}}(a) - E^{\text{GP}}(a)}{\lambda} = \min_{\phi \in \Phi^{\text{GP}}} \langle \phi | S | \phi \rangle. \tag{117}$$

Using $\phi \in \Phi^{\text{GP}}$ as a trial function, we immediately see that $E_{(\lambda S)}^{\text{GP}}(a) \leq E^{\text{GP}}(a) + \lambda\langle\phi|S|\phi\rangle$ for all $\phi \in \Phi^{\text{GP}}$. For the other direction, we use a minimizer of $\mathcal{E}_{(\lambda S)}^{\text{GP}}$ as a trial state for $\mathcal{E}^{\text{GP}}$. As $\lambda \to 0$, this sequence of minimizers will have a subsequence that converges strongly to a minimizer of $\mathcal{E}^{\text{GP}}$. Hence, for some $\phi \in \Phi^{\text{GP}}$, $\lim_{\lambda \searrow 0} \lambda^{-1}(E_{(\lambda S)}^{\text{GP}}(a) - E^{\text{GP}}(a)) \geq \langle\phi|S|\phi\rangle$, which proves our claim. (Note that this argument also proves that the right side of (117) is a true minimum and not merely an infimum.)

We have thus shown that, for every bounded hermitian operator S, and every $\gamma \in \Gamma$,

$$\operatorname{Tr} S\gamma \geq \min_{\phi \in \Phi^{\text{GP}}} \langle \phi | S | \phi \rangle. \tag{118}$$

Replacing S by $-S$, this also implies that $\operatorname{Tr} S\gamma \leq \max_{\phi \in \Phi^{\text{GP}}} \langle\phi|S|\phi\rangle$. Inequality (118) is the key to the proof of statements (ii) and (iii) in Theorem 2.

Let P_n be a rank n projection, and let $P_n\Gamma = \{P_n\gamma P_n : \gamma \in \Gamma\}$. When γ is a bounded operator on $L^2(\mathbb{R}^3)$, $P_n\gamma P_n$ can be identified with an $n \times n$ complex matrix, and hence with a vector in $\mathbb{R}^{2n^2}$. We make this identification (denoted by ι in the following) in order to be able to use finite-dimensional convexity theory (see, e.g., [20]). Note that ι is linear and continuous, and hence the set $B_n = \iota P_n\Gamma = \{\iota P_n\gamma P_n : \gamma \in \Gamma\}$ is a closed convex subset of $\mathbb{R}^{2n^2}$. An *exposed point* [20] of a convex set $\mathcal{C} \subset \mathbb{R}^m$ is an extreme point p of $\mathcal{C}$ with the additional property that there is a tangent plane to $\mathcal{C}$ containing p but containing no other

point of $\mathcal{C}$. (For an example of points that are extreme but not exposed, let $\mathcal{C} \subset \mathbb{R}^2$ be a square with each corner rounded off into a quarter of a circle. The extreme points are all the points on the four quarter-circles, including their endpoints, but the endpoints are not exposed.)

An equivalent way to say this is that an exposed point p in $\mathcal{C} \subset \mathbb{R}^m$ is characterized by the existence of a vector $a \in \mathbb{R}^m$ (a normal to the tangent plane) such that

$$(a, p) \leq (a, b) \quad \text{for all } b \in \mathcal{C} , \tag{119}$$

with equality *if and only if* $b = p$. (Here, $(\cdot, \cdot)$ denotes the standard inner product in $\mathbb{R}^m$.)

For a fixed n, an exposed point of $B_n \subset \mathbb{R}^{2n^2}$ corresponds to some $P_n \widetilde{\gamma} P_n \in P_n \Gamma$. This density matrix $\widetilde{\gamma}$ may not be unique and it may depend on n, but this is of no concern to us.

We note that our space of density matrices is a complex space and, therefore, we have to translate (119) to this setting. For any two bounded operators γ, γ' (not necessarily in Γ), the real inner product $(\cdot, \cdot)$ becomes

$$(\iota P_n \gamma P_n, \iota P_n \gamma' P_n) = \Re \operatorname{Tr}(P_n \gamma^\dagger P_n \gamma') , \tag{120}$$

where $\gamma^\dagger$ is the adjoint of γ. Translated to our original space, this means that if $P_n \widetilde{\gamma} P_n$ is an exposed point of $P_n \Gamma$, then there exists an operator S (with $P_n S P_n = S$) such that

$$\Re \operatorname{Tr} S \widetilde{\gamma} \leq \Re \operatorname{Tr} S \gamma \quad \text{for all } \gamma \in \Gamma , \tag{121}$$

or, equivalently, there exists a *hermitian* S such that

$$\operatorname{Tr} S \widetilde{\gamma} \leq \operatorname{Tr} S \gamma \quad \text{for all } \gamma \in \Gamma . \tag{122}$$

Note that, by definition, equality holds in (122) if and only if $P_n \widetilde{\gamma} P_n = P_n \gamma P_n$. We now use inequality (122), with $\gamma = |\phi\rangle\langle\phi|$, where $\phi \in \Phi^{\mathrm{GP}}$ minimizes $\langle\phi|S|\phi\rangle$ among all GP minimizers. We know from Step 3 that this γ is an element of Γ. The inequalities (118) (applied to $\widetilde{\gamma}$) and (122) for this special choice of γ together imply that there is actually *equality* in this case, and thus that $P_n \widetilde{\gamma} P_n = P_n |\phi\rangle\langle\phi| P_n$. That is, all exposed points of $P_n \Gamma$ are of the form $P_n |\phi\rangle\langle\phi| P_n$, with $\phi \in \Phi^{\mathrm{GP}}$.

We can go further and conclude that *all* extreme points in $P_n \Gamma$ are of this form, not only the exposed points. This follows from the fact that the set of GP minimizers is closed, together with Straszewicz's Theorem [20, Thm. 18.6] which states that the exposed points are a dense subset of the extreme points.

Carathéodory's Theorem [20, Thm. 17.1] implies that every $P_n \gamma P_n \in P_n \Gamma$ can be written as a convex combination of $2n^2 + 1$ extreme points. That is, there exist $\lambda_i \geq 0$ with $\sum_i \lambda_i = 1$ such that

$$P_n \gamma P_n = P_n \left(\sum_{i=1}^{2n^2+1} \lambda_i |\phi_i\rangle\langle\phi_i| \right) P_n , \tag{123}$$

with $\phi_i \in \Phi^{\mathrm{GP}}$ for all i. This equation defines an atomic (i.e., point) measure $d\mu_n(\phi)$ supported on the (compact) space of projections onto GP minimizers. Let us provisionally call this space Δ, with the intention of showing that $\Gamma_{\mathrm{ext}} = \Delta$.

For every ψ with $P_n\psi = \psi$ we have thus shown that

$$\langle\psi|\gamma|\psi\rangle = \int_\Delta d\mu_n(\phi)|\langle\psi|\phi\rangle|^2 \qquad \text{with} \qquad \int_\Delta d\mu_n(\phi) = 1 \, . \tag{124}$$

To complete the proof of Theorem 2 we wish to take the limit $n \to \infty$ in (124). We choose P_n in such a way that P_n converges strongly to the identity as $n \to \infty$. The sequence $d\mu_n$ has a subsequence that converges weakly to some measure $d\mu$ with $\int_\Delta d\mu = 1$ (see [4, vol. 1, Thm. 12.7 and 12.10]). This implies that, for ψ in a dense subset of $L^2(\mathbb{R}^3)$ (namely, those ψ for which $P_n\psi = \psi$ for some n),

$$\langle\psi|\gamma|\psi\rangle = \int_\Delta d\mu(\phi)|\langle\psi|\phi\rangle|^2 \qquad \text{with} \qquad \int_\Delta d\mu(\phi) = 1 \, . \tag{125}$$

Since (125) holds for a dense set of ψ, it actually holds for all ψ by continuity. That is, $\gamma = \int_\Delta d\mu(\phi)|\phi\rangle\langle\phi|$ in the weak sense.

Note that there is a representation (125) for $\gamma \in \Gamma_{\text{ext}}$ (since there is such a representation for all $\gamma \in \Gamma$). It is not hard to see that for an extreme γ the corresponding Borel measure $d\mu$ must be an atomic measure at a single point in Δ. Another way to say this is that $\Gamma_{\text{ext}} \subset \Delta$, which is exactly part (ii) of Theorem 2 (since we have already proved in Step 3 that $\Delta \subset \Gamma_{\text{ext}}$).

Part (iii) of Theorem 2 follows from (125), together with part (ii). This completes the proof of Theorem 2.

We conclude with the direct proof of (11), which was promised just after the statement of Theorem 2. We start with (123) and choose P_n to be the projection onto the largest n eigenvalues of γ, with n large enough so that $\text{Tr}\,|\gamma - P_n\gamma P_n| < \varepsilon^2/8$. We now denote $P_n = P$, $1 - P_n = Q$ and $B = \sum_i \lambda_i|\phi_i\rangle\langle\phi_i|$. From (123) (and a little algebra) we learn that $\gamma - B = Q(\gamma - B)Q - QBP - PBQ$. Thus $\text{Tr}\,|\gamma - B| \leq \text{Tr}\,(|Q\gamma Q| + |QBQ| + 2|QBP|)$. Obviously, $\text{Tr}\,Q\gamma Q < \varepsilon^2/8$ and since $\text{Tr}\,B = \text{Tr}\,\gamma = 1$, we also have $\text{Tr}\,|QBQ| = \text{Tr}\,QBQ = \text{Tr}\,(1 - P)B = \text{Tr}\,(1 - P)\gamma = \text{Tr}\,Q\gamma Q < \varepsilon^2/8$. The remaining term can be bounded, using Schwarz's inequality, by $(\text{Tr}\,QBQ)^{1/2}(\text{Tr}\,PBP)^{1/2} < \varepsilon/\sqrt{8}$. This proves (11).

Appendix: Heat Kernel Estimates

In this appendix we derive an upper bound on the heat kernel for a general Schrödinger operator. This bound will show, in particular, that for any $s > 0$ and α large enough (depending on s)

$$\text{Tr}\,|x|^s e^{\alpha(\Delta - V)} < \infty \tag{126}$$

if $V(x) \geq C_1 \ln(|x|) - C_2$ for some constants $C_1 > 0$ and C_2. This property was used in the proof of Theorem 1. (Actually, in the proof of Theorem 1 we used only the cases $s = 2$ and $s = 4$ (see Step 4 of Sect. 2) because we assumed $A = \frac{1}{2}\Omega \wedge x$, but (126) permits the inclusion of a magnetic field with polynomial growth of A.)

Our bound on the heat kernel follows an idea of Symanzik [26]. Using the Feynman-Kac formula for the integral kernel, we can write

$$e^{\alpha(\Delta-V)}(x,y) = \int d\mu_{x,y}(\omega) \exp\left(-\int_0^\alpha ds\, V(\omega(s))\right), \tag{127}$$

where $d\mu_{x,y}$ denotes the conditional Wiener measure for paths ω going from x to y in time α. By Jensen's inequality we have, for any given path ω,

$$\exp\left(-\int_0^\alpha ds\, V(\omega(s))\right) \leq \frac{1}{\alpha}\int_0^\alpha ds\, \exp\left(-\alpha V(\omega(s))\right). \tag{128}$$

Therefore (using Fubini's Theorem)

$$e^{\alpha(\Delta-V)}(x,y) \leq \frac{1}{\alpha}\int_0^\alpha ds \int d\mu_{x,y}(\omega)\exp\left(-\alpha V(\omega(s))\right)$$

$$= \frac{1}{\alpha}\int_0^\alpha ds\,\left\{e^{s\Delta}e^{-\alpha V}e^{(\alpha-s)\Delta}\right\}(x,y). \tag{129}$$

To evaluate the trace in (126), we only need the heat kernel on the diagonal, i.e., for $x=y$. The integral kernel of $e^{t\Delta}$ is given by

$$j_t(x-y) \equiv \frac{1}{(4\pi t)^{3/2}}e^{-|x-y|^2/4t}, \tag{130}$$

which leads to

$$\left\{e^{s\Delta}e^{-\alpha V}e^{(\alpha-s)\Delta}\right\}(x,x) = \frac{1}{(4\pi)^3}\frac{1}{(t\alpha)^{3/2}}\int_{\mathbb{R}^3} dy\, e^{-\alpha V(y)}\exp\left(-|x-y|^2/4t\right), \tag{131}$$

where t is defined by $1/t \equiv 1/s + 1/(\alpha-s)$.

Let us change the integration variable from s to t, and introduce the function

$$h_\alpha(x) = \frac{2}{\alpha}\int_0^{\alpha/4} dt\,\frac{1}{\sqrt{1-4t/\alpha}}\,j_t(x). \tag{132}$$

Then the bound (129) yields

$$e^{\alpha(\Delta-V)}(x,x) \leq \frac{1}{(4\pi\alpha)^{3/2}}\left(e^{-\alpha V}*h_\alpha\right)(x), \tag{133}$$

with $*$ denoting convolution. Note that $\int h_\alpha(x)dx = 1$. It is easy to see that $h_\alpha(x) \sim \exp(-|x|^2/\alpha)$ for large $|x|$. Hence, if $V(x)$ increases logarithmically with $|x|$, we see that the diagonal of the heat kernel decays at least as $|x|^{-\text{const.}\,\alpha}$ for large $|x|$. Thus, we can choose α large enough to ensure that (126) is finite.

For the proof of Theorem 2 it is necessary to extend this result to the case where $-\Delta+V$ is replaced by $-\Delta+V+K$, with K a finite rank operator. As explained there, we can restrict ourselves to the case when K has exponentially decaying eigenfunctions. I.e., we can assume that the kernel of K, which we denote by $K(x,y)$, satisfies a bound

$$K(x,y) \leq Be^{-D(|x|+|y|)} \tag{134}$$

for some constants $B > 0$ and $D > 0$. Again we want to show that, for any $s > 0$ and α large enough (depending on s),

$$\operatorname{Tr} |x|^s e^{\alpha(\Delta - V - K)} < \infty \tag{135}$$

if $V(x) \geq C_1 \ln(|x|) - C_2$ for some constants $C_1 > 0$ and C_2.

With the notation $L_t = e^{t(\Delta - V)}$, we can use the Dyson expansion to write

$$e^{\alpha(\Delta - V - K)} = L_\alpha + \sum_{n \geq 1} (-1)^n \int_{\sum_i t_i = \alpha} dt_0 dt_1 \cdots dt_n \, L_{t_0} K L_{t_1} K \cdots K L_{t_n} . \tag{136}$$

We have already derived an upper bound on the kernel of L_α above. The kernel of the terms for $n \geq 1$ in the sum can be bounded as follows. First of all, the Feynman-Kac formula tells us that since $V \geq 0$ we have the inequality $L_t(x, y) \leq j_t(x - y)$ for the kernel of L_t. Moreover, using (134) and denoting by Φ the function $\Phi(x) = \sqrt{B} e^{-D|x|}$, we have

$$\left| \left(L_{t_0} K L_{t_1} K \cdots K L_{t_n} \right)(x, y) \right| \leq j_{t_0} * \Phi(x) \prod_{i=1}^{n-1} \langle \Phi | L_{t_i} | \Phi \rangle \, j_{t_n} * \Phi(y) . \tag{137}$$

Since $L_t \leq \mathbb{I}$, we have $\langle \Phi | L_{t_i} | \Phi \rangle \leq \|\Phi\|_2^2$. Denoting

$$\xi_\alpha(x) = \|\Phi\|_2^{-1} \sup_{0 < t < \alpha} j_t * \Phi(x) , \tag{138}$$

we thus have

$$\left| \left(L_{t_0} K L_{t_1} K \cdots K L_{t_n} \right)(x, y) \right| \leq \xi_\alpha(x) \xi_\alpha(y) \|\Phi\|_2^{2n} . \tag{139}$$

The integral over the simplex in (136) yields a factor $\alpha^n / n!$, and hence

$$\left| e^{\alpha(\Delta - V - K)}(x, y) \right| \leq e^{\alpha(\Delta - V)}(x, y) + \left(e^{\alpha \|\Phi\|_2^2} - 1 \right) \xi_\alpha(x) \xi_\alpha(y) . \tag{140}$$

Since ξ_α decays exponentially for large $|x|$ this proves our claim (135).

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